The Art & Science of Beauty

Cosmetic Esters

The Infinite World of Esters

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Preface

Over the years, esters have become an increasingly important class of compounds in the personal care market. The selection of the proper ester for use in a specific formulation has become a more complicated choice, as there are more and more esters to choose from. We at Phoenix Chemical believe that only when an educated choice is made will there be an opportunity to make the most cosmetically elegant formulation. This book was written to provide information to the formulator of personal care products to aid in making that educated choice.

Chapter 1
Raw Materials

1.a. Natural Triglycerides

Oils, Fats, Waxes, and Butters

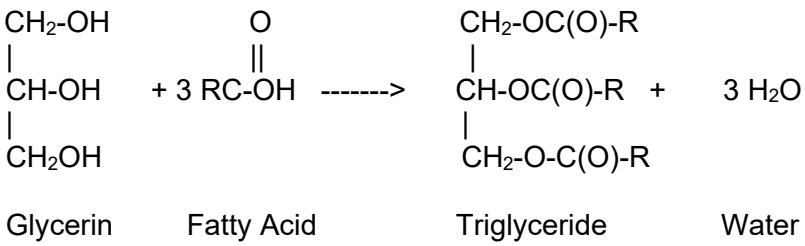
The terms oils, fats, waxes, and butters, have frequently and incorrectly been interchangeably used over the years. Fats have a titer point over 40.5°C, oils have a titer point below 40.5°C. Butters have a titer point below 40.5°C but above 20°C. Oils are liquid at room temperature and the word "oil" is now used to describe any compound that is liquid and is insoluble in water. Butters, oils, and fats are all triglycerides. As a result, jojoba, for example, is referred to as an oil, despite the fact that it is really a liquid wax, a mixture of C_{20} to C_{22} unsaturated esters.

Because oils, fats, butters and waxes are complex mixtures of homologues of similar chemical structures, it is difficult to obtain a true melting point. As the lower molecular weight fractions melt, they act as solvents to dissolve the higher molecular weight products. This results in a very wide melting "range" for these compounds. For this reason, titer point is generally determined on fats, oils, waxes and butters.

The titer is defined as the re-solidification point of the melted oil, fat, butter or wax. The procedure is to heat the product to be tested until it is completely liquid, then to slowly cool with stirring. This is done until the temperature stays constant for 30 seconds, or begins to rise. The titer point is the highest temperature indicated by this rise.[1]

Triglycerides

Triglycerides are the tri-esters of glycerin with three equivalents of an organic fatty acid. Fatty acids are defined as those acids having alkyl or alkylene groups with carbon chain lengths C-5 and higher. The reaction is as follows:

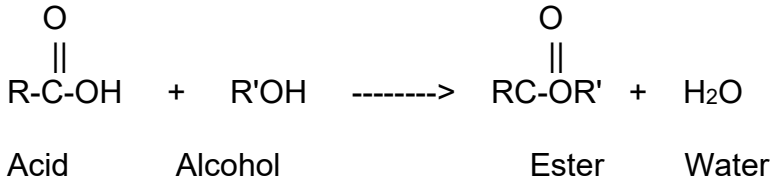


When the triglyceride is saponified to make a surfactant, such as soap, glycerin is liberated. When a wax is saponified, a fatty alcohol is liberated. This makes the type of products that can be made using the two types of materials quite different. Saponification is a general term to define the chemical reaction that breaks the ester linkage. Glycerine, produced as a by-product of saponification is water soluble (hydrophilic) and fatty insoluble (lipophilic). The fatty alcohol produced as a by-product of the saponification of a wax is water insoluble and generally fatty soluble.

Wax Esters

Wax esters are defined as esters of long chained acids that have been reacted with long chain alcohols. Other chemicals are called waxes if they possess tactile properties similar to a true wax such as beeswax. Waxes are widely used in lipstick, make-up, mascara, and solid cosmetic products where structure is necessary to their application.

Wax esters have two fatty groups. One is contained in the alcohol portion of the molecule; the other is in the acid group. Esters are synthesized by the reaction of an organic acid with and an organic alcohol. Esterification is the reverse of saponification, in that ester linkages are formed.



It is necessary to continuously remove by-product water from any esterification process in order to move the reaction toward the formation of the ester.

In the saponification process not only is the fatty alcohol that is formed during saponification water insoluble, many naturally occurring waxes also contain other components, like hydrocarbon resins, which are likewise water insoluble and quite inert to chemical reaction. This needs to be considered during saponification when using these materials.

PCPC (Personal Care Product Council) Nomenclature

PCPC now requires the genus and species of the plants or insects that produce a given wax, oil, butter or fat and all products which are derived from the various oils, fats, butters and waxes. This is due, in part, to the European Union's use of the Latin names for ingredient listings. This information is very helpful to the formulator in understanding the source of the fatty portion of the surfactant.

CLASS I – Animal-Derived Products Rich in Carbon Chain Lengths below C18

Number	Name	Source	CAS Number	Predominant Species
1	Milk Fat	*Cow's Milk*	8029-34-3	C16 Triglyceride

CLASS II – Animal-Derived Products Rich in C_{18} Unsaturated Carbon Chain Lengths

Number	Name	Source	CAS Number	Predominant Species
1	Tallow	*Animal Fat*	61789-13-7	C18:1 Triglyceride
2	Japan Wax	*Rhus Succedanes*	8001-13-6	C16 Wax

CLASS III – Animal-Derived Products Rich in Carbon Chain Lengths Greater than C18

Number	Name	Source	CAS Number	Predominant Species
1	Beeswax	*Cera Alba*	8006-40-4	C26 Wax
2	Shellac Wax	*Shellac Cera*	97766-50-2	C30 Wax

CLASS IV – Plant-Derived Products Rich in Carbon Chain Lengths Below C18

Number	Name	Source	CAS Number	Predominant Species
1	Coconut Oil	*Cocous Nucifera*	8001-31-8	C12 Triglyceride
2	Babassu Oil	*Orbignya Olefera*	91078-92-1	C12 Triglyceride
3	Palm Kernel Oil	*Elaeis Guineenis*	8023-79-8	C12 Triglyceride

CLASS V – Plant-Derived Products Rich in C18 Unsaturated Chain Lengths

Number	Name	Source	CAS Number	Predominant Species
1	Soybean Oil	*Gycerib Soja*	8001-22-7	C18:2 Triglyceride
2	Peanut Oil	*Arachis Hypogaea*	8002-03-7	C18:1 Triglyceride
3	Corn Oil	*Zea Mays*	8001-30-7	C18:1 Triglyceride
4	Sunflower Seed Oil	*Helanthus Annus*	8001-21-6	C18:2 Triglyceride
5	Grape Seed Oil	*Vitis Vinifera*	8024-22-4	C18:3 Triglyceride
6	Safflower Oil	*Carthamus Tinctorius*	8001-23-9	C18:2 Triglyceride
7	Poppy Seed Oil	*Populus Nigra*	8002-11-7	C18:2 Triglyceride
8	Sweet Almond Oil	*Prunnus Amygdalus Dulcis*	8007-69-0	C18:1 Triglyceride
9	Hazelnut Oil	*Corylus Americana*	84012-21-5	C18:1 Triglyceride
10	Walnut Oil	*Juglans Regia*	8024-00-2	C18:2 Triglyceride
11	Olive Oil	*Olea Europasa*	8001-25-0	C18:1 Triglyceride
12	Avocado Oil	*Persea Gratissima*	8024-32-6	C18:1 Triglyceride
13	Sesame Oil	*Sesamum Indicum*	8008-74-0	C18:1 Triglyceride
14	Tall Oil	*Tallol*	8002-26-4	C18:1 Fatty Acid
15	Cottonseed Oil	*Gopssypium*	8001-29-4	C18:2 Triglyceride
16	Palm Oil	*Elaesis Guineensis*	8002-75-3	C18:1 Triglyceride
17	Rice Bran Oil	*Oryza Sativa*	68553-81-1	C18:1 Triglyceride
18	Canola Oil	*Canola*	8002-13-9	C18:1 Triglyceride
19	Apricot Kernel Oil	*Prunus Armeniaca*	72869-69-3	C16 Triglyceride
20	Shea Butter	*Butyrospermum Parkii*	977026-99-5	C18 Triglyceride
21	Wheat Germ Oil	*Triticum Vulgare*	8006-95-9	C18:2 Triglyceride
22	Illipe Butter	*Bassia Latifola*	68424-60-2	C18 Triglyceride

CLASS VI – Plant-Derived Products Rich in Carbon Chain Lengths Greater Than C-18

Number	Name	Source	CAS Number	Predominant Species
1	Meadowfoam Seed Oil	*Limnanthes Alba*	153065-40-8	C20:1 Triglyceride
2	Rapeseed Oil	*Brassica Capmestris*	8002-13-9	C22:1 Triglyceride

CLASS VII – Products having unusual carbon chain lengths or composition

Number	Name	Source	CAS Number	Predominant Species
1	Borage Seed Oil	*Borago officinalis*	8401201608	C18:3 (n=6) Triglyceride
2	Linseed Oil	*Linum usitatissimum*	8001-26-1	C18:3 (cong) triglyceride
3	Castor Oil	*Ricinus communis*	8001-79-4	C18:1 OH triglyceride
4	Veronia Oil	*Veronia galamensis*	169360-96-7	C18 epoxy triglyceride

5	Tung Oil	*Aleurites fordii*	8001-20-5	C13:3 (cong) triglyceride
6	Jojoba Oil	*Buxus chinensis*	61789-91-1	C20 ester
7	Candelilla Wax	*Euphorbia cera*	8006-44-8	C31 hydrocarbon
8	Ongokea Oil	*Ongokea gore*		C18:3 acetylenic

Nature has provided a plethora of materials that are potentially useful in the personal care applications. The type and source of natural raw materials is a major variable to be considered by the formulator in making new cosmetic products. The formulator needs to know some basic information on the sources and chemistries of these raw materials to make informed decisions on product formulation. Not only performance, but also as importantly, cost and label copy are determined by the selection of oils and waxes, both per se and in surfactant molecules.

Chemists are always interested in the composition of natural oils and the source. The following is offered as a general overview of the topic. A book on the chemistry of triglycerides is available on the web free of charge[1]. Triglycerides can be classified into three groups as shown.

[1]*Primary Ingredients* by O'Lenick, Anthony J., Steinberg, David and Klein Kenneth, 1998.

1.b. Refining

The process that allows for the transformation of a plant seed into clear low odor oil suitable for cosmetic use is a process that we generally take for granted. The plant chosen for use as well as the processing used determines the properties of the oil.

The oils covered in this article are referred to as "vegetable oil." This differentiates them from "essential oils" which are often pleasant-smelling oils that are steamed out of a variety of plant parts, including flowers, leaves, peels and some seeds. Essential oils are not triglycerides like the vegetable oils but usually "isoprenoids", that is they come from a different chemical pathway in plants.

Isoprenoids are among the most diverse group of compounds synthesized by biological systems. It has been estimated that there are approximately 22,000 known isoprenoids, which includes terpenoids and carotenoids. It can be readily seen that essential oils are far removed in chemical composition from triglycerides. Plants store vegetable oils (triglycerides) as energy sources for seeds when they germinate**.**

Steam works well to extract essential oils like coriander oil but not for triglyceride oils. Triglyceride and wax ester oils can be squeezed out of seeds using a turning screw that presses the mashed-up seed against a metal barrel with slits in the side. The oil and some fine particles squeeze out the narrow slits. This operation would be called an oil expeller or seed oil press. The oil from the seed oil press can be filtered and called "virgin" oil, especially if it isn't heated up to get more oil out. The oil from the seed oil press can also be called crude oil. Alternatively, oil can be dissolved in solvent, followed by evaporation of the solvent leaving the extracted oil.

Often, seeds are flaked to increase surface area. The seeds are processed into thin flakes before pressing or solvent extraction. The flaking improves oil yield by breaking open the small oil pockets in the seeds. Sometimes the seeds are heated before flaking so that the proteins in the seed won't break down the oil or other components in the seed. The preheating is also called preconditioning. The oil comes out more easily if it is hot, but too much heat damages the oil quality.

Sometimes the seeds are crushed and formed into pieces called "collets" that have lots of holes or openings. This step also is done before solvent extraction to make the oil easier to flow. Solvent extracted oil with some solvent still in it is called the "miscella."

Crude oil can be good enough for chemical uses. However, well-filtered "virgin" oil is recommended for cosmetic use. This is accomplished by keeping the oil cold and filtering it to remove any solid waxes that might crystallize out in a process called "winterization".

Many cosmetics applications require cold-pressed, virgin oil. On the other hand, some seeds are too low in oil to economically remove the oil by pressing. In any case, once you have the crude oil, you can move onto refining.

Refining is done by filtering the oil through clay or silica (like fine sand) which can remove color. In an operation called "degumming" alkali dissolved in water is added to the oil. Some ingredients, especially fatty acids go into the water or settle out or are filtered out. Finally, steam can be passed through the oil to remove odor in an operation called deodorization. This step also breaks down oxygen attached to the oil, which might lower oil quality.

Hopefully, after all of this refining the oil is light in color, has no odor, no oxygen breakdown products and no solid wax. The amount of oil you have left after refining is often related to the amount of crude oil you started with or to the amount of oil in the seed by the "yield" of oil from each step in the process.

The yield of refined oil may be significantly less than the crude oil put into the process. This explains why refined oils are more expensive.

The oils that are commonly used in cosmetic products are complex mixtures of different triglycerides, but also contain various other components that are useful. For example, olive oil can be processed to contain highly desirable tocopherols. Solvent extraction or steam distillation would remove much of this material. If the oil was in the formulation for the benefit derived from the tocopherols, the potential variations in the processing could have dramatic consequences. The winterizing of oils, that is cooling and filtration of solids from the liquid results in a loss of the higher molecular weight fractions. Many times, it is exactly these fractions that provide the unique skin feel or conditioning to the product. It should be clear that the different processes used in the preparation of an oil may be critical to functionality.

1. c. Fractionation

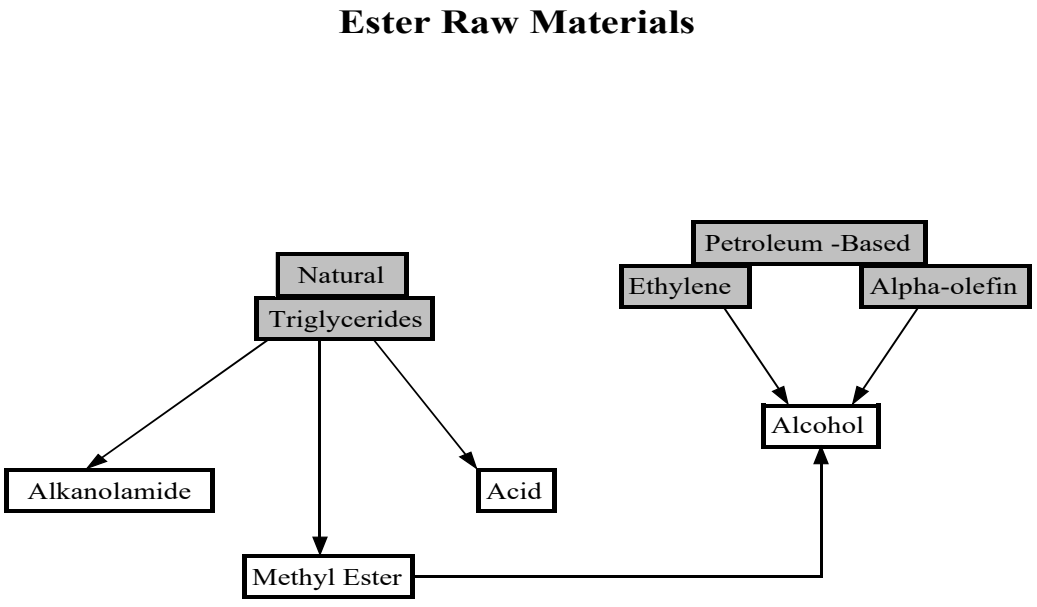
Methyl esters made from oils are fractionated into products containing discrete alkyl groups. This is done by distillation.

Methyl Esters

Triglycerides may be easily turned into methyl esters by reaction with methanol and catalyst. Base catalysts are preferred. As the reaction proceeds, the reaction mixture turns hazy as glycerin is liberated. Once complete, the excess methanol is distilled off, glycerin removed from the bottom after it settles and the methyl ester is distilled into its fractions.

The methyl ester formed by the reaction, if not distilled is still referred to by the oil name (for example methyl cocoate). However, once fractionated the material is named by carbon distribution. Methyl cocoate is fractionated into methyl laurate, methyl myristate and so on. The triglyceride source is lost in the name of the methyl ester. The names for the common alkyl groups are given below. Distillation is a major operation used to fractionate the methyl ester mixture obtained from oils into specific defined methyl esters having the desired alkyl groups.

1. d. Reduction



Fatty Acids

Fatty acids are also available that have specific "cuts". They include acids having a wide distribution, like coco fatty acid (having essentially the same distribution as the oil). They also include very specific cuts having a composition of a single fatty acid. One of the most confusing aspects of dealing with fatty acids is the nomenclature**.**

Commonly Used Fatty Acid Nomenclature[2]

Designation	Name	Formula
C6	*Caproic acid*	$C_6H_{12}O_2$
C8	*Caprylic acid*	$C_8H_{16}O_2$
C10	*Capric acid*	$C_{10}H_{20}O_2$
C12	*Lauric acid*	$C_{12}H_{24}O_2$
C12:1	*Lauroleic acid*	$C_{12}H_{22}O_2$
C14	*Myristic acid*	$C_{14}H_{28}O_2$
C14:1	*Myristoleic acid*	$C_{14}H_{26}O_2$
C16	*Palmitic acid*	$C_{16}H_{32}O_2$
C16:1	*Palmitoleic acid*	$C_{16}H_{30}O_2$
C18	*Stearic acid*	$C_{18}H_{36}O_2$
C18:1	*Oleic acid*	$C_{18}H_{34}O_2$
C18:2	*Linoleic acid*	$C_{18}H_{32}O_2$
C18:3	*Linolenic acid*	$C_{18}H_{30}O_2$
C20	*Arachidic acid*	$C_{20}H_{40}O_2$
C20:1	*Gadoleic acid*	$C_{20}H_{38}O_2$
C22	*Behenic acid*	$C_{22}H_{44}O_2$
C22:1	*Erucic acid*	$C_{22}H_{42}O_2$
C22:2	*Clupanodinic acid*	$C_{22}H_{40}O_2$
C24	*Lignoceric acid*	$C_{24}H_{48}O_2$
C26	*Cerotic acid*	$C_{26}H_{52}O_2$
C28	*Montanic acid*	$C_{28}H_{56}O_2$
C30	*Myricic acid*	$C_{30}H_{60}O_2$
C32	*Lacceroic acid*	$C_{32}H_{64}O_2$
C34	*Geddic acid*	$C_{34}H_{68}O_2$

There are a wide range of products that are produced by utilizing the various fatty acids and methyl esters made using the processes described above.

[2]O'Lenick, Anthony J., *Surfactants Chemistry and Properties* 1999, Allured Publishing Corporation p. 13-15.

Chapter 2

Naturally Occurring Esters

There are a number of naturally occurring esters of which the reader should be aware.

These are described below.

1. Beeswax (Cera Alba)
2. Jojoba Oil (aka Jojoba Wax; Simmondsia Chinesis)
3. Shea Butter (Shorea Stenoptera L.)

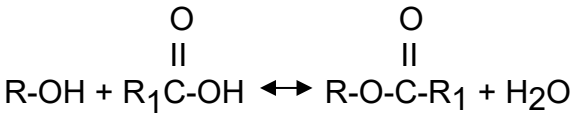
These esters are often synthetically derived either as neat chemical equivalents to naturally occurring esters and oils such as PELEMOL BB (INCI: Behenyl Behnate) a component of Hydrogenated Jojoba Oil or as functional equivalent such as PELEMOL OE (INCI: Oleyl Erucate) for Jojob Oil. Chemically different esters from naturally occurring esters are synthesized to emulate physical characteristics such as melting point and solubility profiles as exemplified by PELEMOL TT (INCI: Tribehenin (and) Caprylic/Capric Triglyceride) or BIOGEL Soybean Oil/FH (INCI: Hydrogenated Soybean Oil), a synthesized substitute for Beeswax.

Chapter 3

Ester Technology

By definition: An **Ester** is the reaction product of an organic acid with an organic alcohol or glycol.

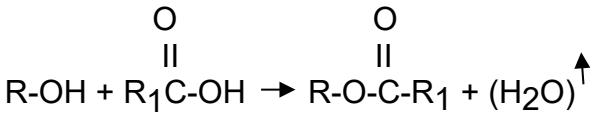
This reaction can be illustrated thus:



Where R and R1 can be same or different alkyl or aryl or aryl-alkyl groups.

Please note that the reaction is reversible - esters can hydrolyze back to their original components

Thus, there is the need to remove water in order to unbalance the reaction toward the ester side. With perfectly efficient removal of water, the reaction can be illustrated like this:



Since there is no perfect method of water removal, and some esters are harder to react than others, we now have a bit of art mixed with our science.

3.1 HOW ARE ESTERS PRODUCED?

Esters come in various sizes ranging from two carbons (methyl formate) to over 100 carbons in length, with no end in sight.

They are produced in several ways. here are a few:

Endothermically (heating the components to a temperature that initiates and continues the reaction). The trick with endothermic reactions is taking care not to "throw away the baby with the bath water." The temperatures required to drive many esterification reactions also sharply increases the vapor pressure of one or more of the reactants. Add a little nitrogen sparge * and you'll find a portion of at least one of your reactants merrily tagging along with the water vapor to end up in the receiver. So much for stoichiometry! Hurrah for Murphy!

* A nitrogen blanket or sparge is a must for most reactions. It's amazing what the introduction of a little air (oxygen) can do to the color of the final product

Catalytically (addition of a substance that initiates/sustains the reaction without modification to itself.) Catalytically induced reactions are generally faster and more efficient than those driven by heat alone. However, use of a catalyst means another raw material to be added (usually expensive, too.) Sometimes an extra step is required to neutralize or remove it at the end of the reaction to make the product acceptable to the customer; who is, after all, the final authority. The way catalysts work is part of the mystique and black magic of esterification. Such knowledge is best left in the gnarled hands of theoreticians wearing high, conical hats. For the rest of us, it's mostly *educated* trial and error for R&D folks to determine which specific catalyst works best in our particular reaction (hey, if we knew what we were doing, it wouldn't be called **research**, right?) However, such knowledge, once applied, becomes part of the wisdom of the senior chemist. There is quite a list catalyst types to choose from:

Acid catalysis is probably the oldest type used in esterification. After all, one of the reactants is a free acid; albeit not usually a strong one. Although Sulfuric Acid works well, and has been widely used in the past, it does cause color problems. In the last 30 or 40 years, Sulfonic acids such as Methanesulfonic or p-Toluenesulfonic Acids have been successfully used in a great variety of esterification reactions. Even with these acids, color development can still be a problem.

Alkaline catalysis, usually in the form of metal hydroxides such as Sodium, Potassium or Calcium Hydroxide can be used for esterification, transesterification and alkoxylation. These, too, must be used carefully to avoid color problems.
Just as an aside, do you recall how our ancient ancestors discovered that animal fat dripping onto the ashes of the cooking fire produced that bubbly substance called ***soap***? It's not hard, then, to picture the following reaction steps:

Fatty Acid + Metallic Hydroxide + Fatty Alcohol →

Fatty acid metallic salt (SOAP) + Fatty Alcohol + Water↑ →

Fatty Ester + Metallic Hydroxide

Or (for you technical types):

$$ROOH + KOH(\text{PAR EX.}) + R_1OH \rightarrow$$

$$ROO^-K^+ + R_1OH + H_2O\uparrow \rightarrow$$

$$ROOR_1 + KOH$$

Of course, by definition, a catalyst initiates and/or sustains a reaction without modification to itself. However, if it ends up the same as it started, has it really been modified? And what is the sound of *one* hand clapping?

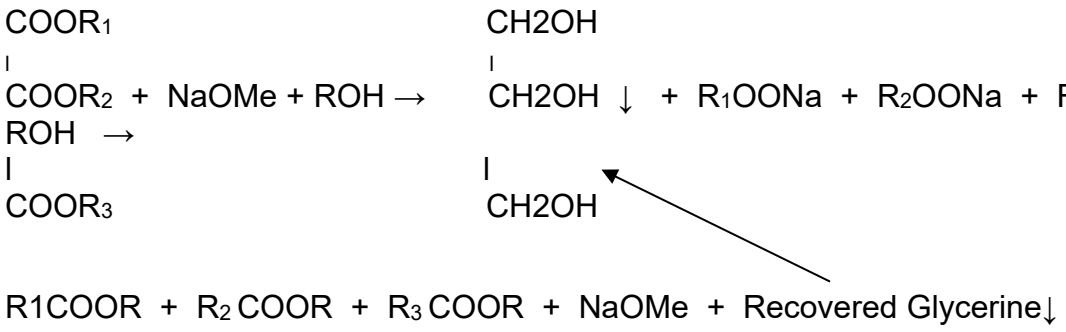
Many **metals** can also drive esterification reactions. Both pure metals and their derived compounds, such as salts, have been used as catalysts. Copper, zinc, tin, iron, aluminum and zirconium are the most commonly used. Care must be taken when using metals since undesirable side reactions can occur resulting in contamination of the final ester.

Organo-metallic compounds are a special class of metal derivatives that are widely used to catalyze esterification. The most common of these are the tin compounds of which a great variety is available. These have proven quite useful, especially in high-temperature reactions.
Examples are: Stannous Oxalate, Stannous Oxide.

Biocatalysis has come a long way in recent years. Enzymes and other bioactives have been specially developed to make and/or break ester bonds at relatively low temperatures in a variety of media. On the positive side, these catalysts are usually bonded to a substrate that makes them reusable for varying periods of time or numbers of batches. On the flip (other) side, they can be quite expensive and so is the technology to utilize them.

Other known esterification catalysts include modified **Zeolites** and special **Ion-exchange Resins**. Another heading might include **Phase Transfer** catalysts, just in case your reactants don't mix very well. These highly specialized molecules consist of crown ethers and their derivatives as well as special cationics and quaternaries. Please be assured that this is, by no means, an exhaustive list. Just as there are yet thousands of plant and insect species yet to be discovered, so too is the field of catalysis. Catalysis is an expanding science and there are yet many catalysts to be discovered.

1. Transesterification is a way of making esters from other esters such as making methyl esters from triglycerides, mono and dialkyl esters from triglycerides or other esters from methyl esters, using longer-chain alcohols. This is a good way of capturing and isolating specific fatty acids from naturally-occurring fats and oils. First, a triglyceride, like coconut oil (vegetable oil) is saponified to yield glycerine and soap (remember the fatty acid-metal salts?) thence to the methyl esters of the individual fatty acids. By fractional distillation, these methyl esters can be separated into individual components, such as Methyl Laurate, Methyl Myristate, Methyl Palmitate, Methyl Oleate, and Methyl Stearate. In turn, these fractions can be transesterified to yield other esters, like Methyl Palmitate to Cetyl Palmitate.
The reactions can be visualized thusly:



The methyl esters can now be recovered, purified and separated from one another to yield pure cuts of FAME (**f**atty **a**cid **m**ethyl **e**ster). These, in turn can be converted into other, value-added products.

2. In **interesterification,** one makes a new product by reacting two or more esters with one another. To illustrate, a **tri**glyceride can be reacted with a **mono**glyceride to yield a **di**glyceride. In some specialized applications two oils with different fatty acid compositions are reacted such that fatty groups are transferred from one oil to the other in a "rearrangement" to yield a new oil with the desired properties.

3. Alkoxylation occurs when reacting fatty acids with ethylene oxide, propylene oxide or butylene oxide, etc. These esters are named according to the alkoxide added, like Ethylene Glycol or Polyethylene Glycol esters; Propylene Glycol or Polypropylene Glycol esters such as PEG-8 Distearate.Similarly although this class of compounds are ether alkoxides can be reacted with fatty alcohols to yield products such as Laureth-9 or Steareth-20. etc. These reactions can of course be carried out with multifunctional organic acids or alcohols to yield corresponding complex esters or ethers. Generally speaking, addition of ethylene oxide will <u>increase</u> water solubility and melting point while propylene oxide <u>decreases</u> water solubility and <u>lowers</u> melting point.

3.2 HOW MANY KINDS OF ESTERS ARE THERE?

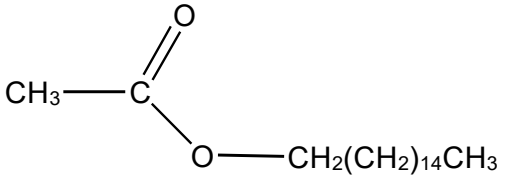
Esters come in many sizes and shapes. Here are a few examples:

Simple Esters - straight chain alcohol and mono-acid:

PELEMOL CA

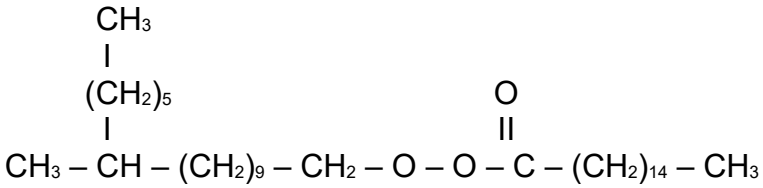
(INCI: Cetyl Acetate)

PELEMOL CA is structurally described as:



Branched Esters - made from branched alcohol, acid or both:

ISOSTEARYL PALMITATE

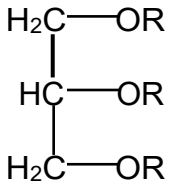


Diesters, Triesters, etc. - from glycols **or** acids with two or more functional groups:

PELEMOL GTIS

(INCI: Triisostearin)

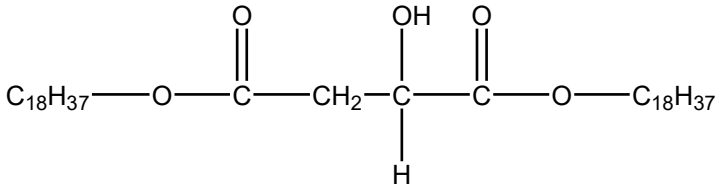
PELEMOL GTIS is structurally described as:



where R = Isostearic Acid

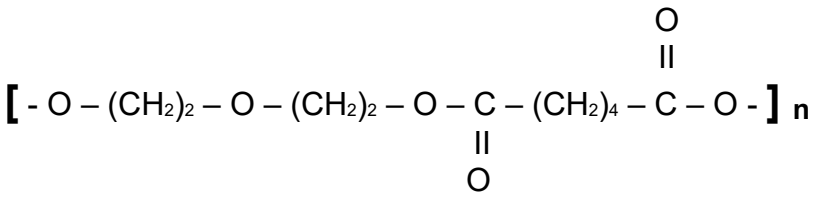
PELEMOL DISM

(INCI: Diisostearyl Malate)



Polyesters - reactions involving polyglycols and polyacids that yield polymeric products:

DIETHYLENE GLYCOL ADIPATE

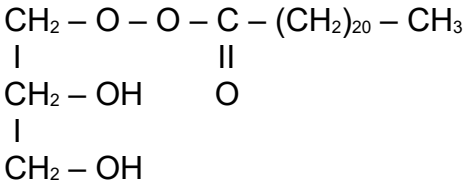


Where n= repeating monomer unit

Partial Esters - non-stoichiometric reactions between polyfunctional components which leave free carboxylic and/or hydroxyl groups. Pelemol GMB (Inci: Glyceryl Behenate) is a classic example of a partial ester.

PELEMOL GMB

(INCI: GLYCERYL BEHENATE)



If you have let your imagination wander as you read this information, you perhaps began to realize that the realm of esters is **not** a "***small, small world***!" In fact, it's quite the opposite. In form, esters range from light, volatile liquids to dense, rocklike solids and everything in between.

3.3 WHAT ARE ESTERS MADE OF?

To even further expand this panorama, we are going to consider some of the raw materials used in making esters. As was mentioned at the beginning of the story, esters are the product of the reaction between an organic acid (think carboxylic group) and an alcohol (think hydroxyl group). These acids and alcohols take many forms so, before we do that, it might alleviate some

confusion if we explain some of the names given to these fatty acids and alcohols so you will recognize them.

Let's use a couple of tables; one for acids and one for alcohols (these terms are used in the broadest sense, as you will see.)

NOMENCLATURE OF COMMONLY USED FATTY ACIDS

# of Carbons	Monoacid	Branched	Diacid	Unsaturated
1	FORMIC METHANOIC			
2	ACETIC ETHANOIC		OXALIC GLYCOLIC	
3	PROPIONIC PROPANOIC		MALONIC TARTRONIC, TARTARIC	ACRYLIC PROPIOLIC
4	BUTYRIC BUTANOIC	ISOBUTYRIC	SUCCINIC, MALIC MALEIC, FUMARIC	METHACRYLIC CROTONIC
5	VALERIC PENTANOIC	PIVALIC ISOVALERIC	GLUTARIC CITRA-, MESACONIC	
6	CAPROIC HEXANOIC		ADIPIC	
7	HEPTANOIC ENANTHIC		PIMELIC	
8	CAPRYLIC OCTANOIC	2-ETHYLHEXANOIC	SUBERIC	
9	PELARGONIC NONANOIC	ISONONANOIC	AZELAIC	
10	CAPRIC DECANOIC	NEODECANOIC	SEBACIC	
11	UNDECANOIC			UNDECENOIC UNDECYLENIC

12	LAURIC DODECANOIC	ISOLAURIC 2-BUTYLOCTANOIC	DODECANEDIOIC	
13	TRIDECANOIC			
14	MYRISTIC TETRADECANOIC			MYRISTOLEIC
NOMENCLATURE OF COMMONLY USED FATTY ACIDS				
15	PENTADECANOIC			
16	PALMITIC HEXADECANOIC	ISOPALMITIC 2-HEXYLDECANOIC		PALMITOLEIC
17	MARGARIC			
18	STEARIC OCTADECANOIC 12- HYDROXYSTEARIC	ISOSTEARIC 2-OCTYLDECANOIC		OLEIC, ELAIDIC LINOLEIC,LINOLENIC RICINOLEIC
20	ARACHIDIC ICOSANOIC			
22	BEHENIC DOCOSANOIC			
24	TETRACOSANOIC	2-DECYLTETRADECANOIC		
32	DOTRIACONTANOIC	OCTADECYLTETRADECANOIC		

So much for the fatty acids, did you count them all? Each one (or more) of the above acids can be reacted with any one (or more) of the following alcohols and glycols:

NOMENCLATURE OF COMMONLY USED ALCOHOLS & GLYCOLS

# of Carbons	**Alcohol**	**Branched**	**Diol**	**Polyol**
1	METHANOL			

2	ETHANOL			
3	PROPANOL	ISOPROPANOL	PROPANEDIOL PROPYLENE GLYCOL	GLYCERINE
4	BUTANOL	ISOBUTANOL SEC./TERT. BUTYL	BUTANEDIOL DIETHYLENE GLYCOL	
5	PENTANOL AMYL ALCOHOL	ISOAMYL ALCOHOL	NEOPENTYL GLYCOL	PENTAERYTHRITOL
NOMENCLATURE OF COMMONLY USED ALCOHOLS & GLYCOLS				
6	CAPROYL ALCOHOL HEXANOL		TRIETHYLENE GLYCOL HEXANEDIOL DIPROPYLENE GLYCOL	TRIMETHYLOLPROPANE DIGLYCEROL SORBITOL, etc.**
7	HEPTANOL			
8	CAPRYLYL ALCOHOL OCTANOL	2-ETHYLHEXANOL 2-OCTANOL	PEG-4 OCTANEDIOL	
9	NONANOL NONYL ALCOHOL	ISONONANOL	TRIPROPYLENE GLYCOL	POLYGLYCERIN-3
10	CAPRYL ALCOHOL DECANOL	ISODECANOL	PEG-5	DIPENTAERYTHRITOL
11	UNDECANOL			
12	LAURYL ALCOHOL DODECANOL	2-BUTYLOCTANOL	DODECANEDIOL PPG-4, PEG-6	POLYGLYCERIN-4 SUCROSE DITRIMETHYLOLPROPANE
13	TRIDECANOL TRIDECYL ALCOHOL			
14	TETRADECANOL MYRISTYL ALCOHOL			
15	PENTADECANOL		PPG-5	POLYGLYCERINE-5 TRIPENTAERYTHRITOL
16	PALMITYL ALCOHOL HEXADECANOL	HEXYLDECANOL HEXADECYL ALCOHOL	PEG-8	
17	HEPTADECANOL			

18	STEARYL ALCOHOL OCTADECANOL	ISOSTEARYL ALCOHOL OCTYLDECANOL	PPG-6 PEG-9	POLYGLYCERIN-6 TRITRIMETHYLOLPROPANE
19	NONADECANOL			
20	ARACHIDYL ALCOHOL ICOSANOL	OCTYLDODECANOL ISOICOSANOL	PEG-10	
22	BEHENYL ALCOHOL DOCOSANOL		PEG-11	
24	TETRACOSANOL	DECYLTETRADECANOL	PPG-8 PEG-12	POLYGLYCERIN-8
NOMENCLATURE OF COMMONLY USED ALCOHOLS & GLYCOLS				
28	OCTACOSANOL	DODECYLHEXADECANOL	PEG-14	
30	TRIACONTANOL		PPG-10 PEG-15	POLYGLYCERIN-10
32	DOTRIACONTANOL	TETRADECYL-OCTADECANOL		
34	TETRATRIACONTANOL	HEXYLDECYL-OCTADECANOL		
36	HEXATRIACONTANOL	CETYLARACHIDOL	PPG-12	
40	TETRACONTANOL		PEG-20	
50	PENTACONTANOL		PEG-25	
100	HECTANOL		PEG-50	

** The sugars Fructose, Glucose and Mannitol are also C_6 polyols.

Please bear in mind that this is by no means an exhaustive compendium, nor is it intended to be a lesson in IUPAC nomenclature. It is only meant to be a handy (I hope) summary of the most familiar compounds. Such materials as aromatic compounds and polyacids (like citric) have been left out of these tables to avoid getting too complicated and the tables too cramped. No offense was meant to our aromatic friends – they will be mentioned later. Now we can get back to the issue at hand – from what raw materials esters are made.

Alcohols, Glycols, Polyols

1. Straight chains (C_2 through C_X.)

OCTANOL

$$CH_3 – (CH_2)_6 – CH_2OH$$

2. Branched chains (C_3 through C_{36})

2-ETHYLHEXANOL

$CH_3 – CH – (CH_2)_3 – CH_2OH$
I
CH_2
I
CH_3

OCTYLDODECYL ALCOHOL *

$CH_3 – CH – (CH_2)_9 – CH_2OH$
I
$(CH_2)_7$
I
CH_3

- Octyldodecyl Alcohol is an example of a **GUERBET** Alcohol. These are synthetic compounds made by joining two straight chains to form a new, branched moiety.

3. Glycols (PEG's, PPG's and other diols):

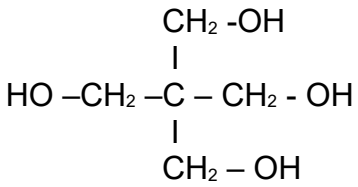
PEG-8 or PEG 400 *

$$H [–O - CH_2 – CH_2 – O – CH_2 – CH_2 –]_8OH$$

* PEG-8 refers to eight moles of Ethylene Oxide, while PEG 400 is the approximate molecular weight.

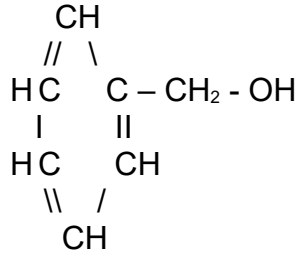
4. Polyglycols (Glycerol, Sorbitol, TMP, PE, etc.)

PENTAERYTHRITOL



5. Aromatics or ring-containing (Benzyl Alcohol, Resorcinol, etc)

BENZYL ALCOHOL

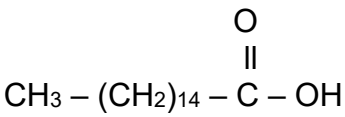


We could go on a while longer and mention some of the biological raw materials like cholesterol or the phytosterols, tocopherols and others. These products have very specialized applications and are essentially esterified in the same way as other alcohols. They are, however, a good deal more complex in structure; and, frankly, I'm just too lazy to draw them.
Having admitted that minor flaw in my character, let's move on to the acid section of our ester components.

Organic Acids

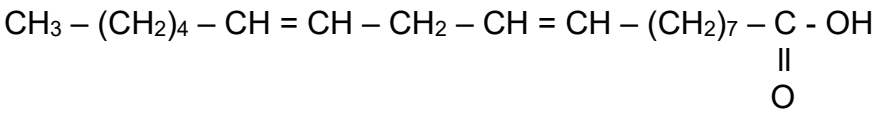
1. Saturated straight chains (lauric, stearic, etc.)

PALMITIC ACID



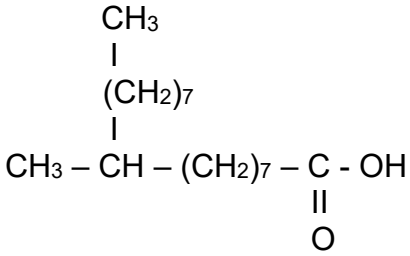
2. Unsaturated straight chains (oleic, erucic, etc)

LINOLEIC ACID



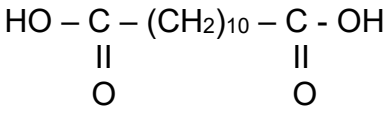
3. Branched chains (2-ethylhexanoic, synthetics)

ISOSTEARIC ACID



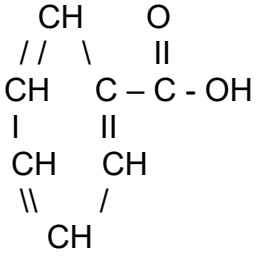
4. Di- and trifunctional acids (adipic, trimellitic, etc.)

DODECANEDIOIC ACID



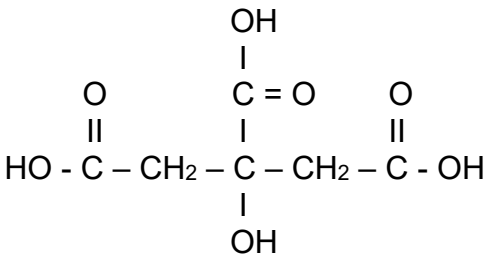
5. Aromatics (benzoic acid, paba, etc.)

BENZOIC ACID



6. Hermaphrodites (my term)- fatty acids that contain both carboxylic and hydroxyl groups (ricinoleic, 12-hydroxystearic, citric, lactic, etc.)

CITRIC ACID



With this plethora of molecules we call esters, it must be obvious by now that there is almost as great a variety of uses and applications for these versatile products. If you are currently using esters in your work, then you know a few of them already.

3.4 WHAT ARE ESTERS USED FOR?

Now that we have discussed the composition of esters and let us try to summarize their myriad of uses (although no one person knows them all).

Ask 100 chemists what esters are used for and the number one response would probably be ***emulsifier***, while the number two answer would likely be ***emollient***. so let us start with those.

Most personal care chemists are quite familiar with the ***HLB System***, which compares the ratios of hydrophilic and lipophilic portions of molecules on a scale of 0 – 20+. Esters, it seems, can both emulsify and be emulsified. The emulsifier, as a rule, has both water-soluble and oil-soluble moieties within its structure. Mono- and diglycerides, Sorbitan esters, Polyglyceryl esters, Ethylene and Polyethylene Glycol (PEG) esters and Neopentyl Glycol-type partial esters are some of the best known on the emulsifier list.

Many other esters function as oils and waxes that leave a smooth, soothing coating on the skin, known as ***emolliency.*** These are the esters that contribute most to the "skin feel" of topical formulations. The most common emollients are the short-chain alcohol esters (Ethyl, Isopropyl,

Butyl, etc.). In recent times, however, liquid to soft wax esters have been developed that exhibit cushiony smoothness and which contain 100 carbons and more.

Among other well-known applications for esters are their uses as ***solubilizers, dispersants*** and ***stabilizers***. Each of these applications, in the end, successfully blends ingredients that would not ordinarily mix (at least, not for long!).

Solublizers help to incorporate an ingredient, such as a fragrance, into a formulation by making a "solution within a solution."
Dispersants, as the name implies, help to evenly disperse an insoluble ingredient (a pigment or TiO_2, for example) into a formulation and keep it there.
Stabilizers are used to maintain the state of a mixture either by physical means (par. ex. viscosity) or chemical means (like a pH buffer).
Please note that none of the resultant mixtures are ***emulsions***. The mechanisms of ***emulsifiers, solubilizers, dispersants*** and ***stabilizers*** differ from one another in various ways. (If our readers are interested, perhaps an exploration of these mechanisms could be the subject of another article.)

Lubricants

Were you aware that the highly acclaimed synthetic motor oil you use in your car is ester-based? The synthetic oil used in aircraft jet engines must be able to withstand very high temperatures and yet have a cloud point of –40 degrees. Guess what? Esters again! These same types of esters find lubricant applications in the textile, metalworking and plastics industries, as well. Many of these lubricants are based on NPG-type glycols esterified with low to medium chain-length fatty acids. The fact that they generally exhibit high smoke and flash points but low cloud and titer points makes them very desirable for high-speed, high temperature, high friction and/or high altitude applications.

Nutritional Aids

Did you know that medium-chain triglycerides (or MCT oils) are digested as *carbohydrates* rather than as fats? In fact, a teaspoon of MCT oil yields more energy to the body more quickly than an equivalent amount of sugar. Is it any wonder, then, that MCT oil is a standard nutritional aid in baby formulas and geriatric supplements? Today, many types of triglycerides and

polyglyceryl esters are especially designed for incorporation into food products to both reduce fat intake (by substituting indigestible molecules) and to supply the "right" fats.

Flavors & Fragrances

There are many "natural" esters that impart a characteristic flavor and/or fragrance to the foods we eat and the pharmaceutical/personal care products we use. Although many of these are produced naturally, we have found ways to synthesize them and even make them better(?) For example, there are esters that smell like limburger or provolone cheeses, some that smell like peaches or bananas, some even "come out smelling like a rose." The majority of these esters are low in molecular weight, which attributes to their volatility.

Other Specialties

Some of the most effective sunscreen products are based on aromatic compounds, many of which are esters.

Remember your ***polyester*** bell-bottom pants? Polyesters are simply highly cross-linked esters that can be extruded into fibers and woven into cloth or carpeting.

Many esters are added to vinyl and other plastics to impart flexibility or, at least, reduce brittleness. In this application they are called ***plasticizers.*** Think about such products as medical equipment (especially tubing), food film, upholstery, flooring, moldings, gasketing, athletic shoes, rainwear, wire insulation, PVC pipe, auto trim, pool and pond liners, roofing systems and so on and so on.

Along these same lines, esters are employed in the plastics, ceramics and glass industries as mold release agents. Before casting, the mold is coated with an ester (usually a high temperature lubricant, as you might guess) to prevent the casting from sticking to the mold. Sometimes, the ester is incorporated in the material to be molded and thus can also act as an internal lubricant or a plasticizer.

In the foundry industry, temporary sand molds are made by mixing glyceryl acetates and sodium silicate with the sand, forming the mold and letting it harden. Set times can be adjusted from a few minutes to a couple of hours. When finished with the mold, it can simply be pulverized back

into sand and reused. This same technique can be used to form temporary, solid walls in construction trenches, tunnels, etc.

Interesterified triglycerides are used to "temper" chocolate candies to prevent *syneuresis* or "weeping."

Esters are used in deodorant and antiperspirant stick formulations as "anti-whitening" agents.

I'll bet you never heard of a "***scrooping agent."*** The next time you have need to open a box of absorbent cotton, squeeze a little ball of it between your fingers. With some brands, if you hold it up to your ear, you can even hear the "*scroop, scroop"* as you flex the cotton ball. Processed cotton fibers are typically quite soft and limp. An ester, known as a ***"scrooping agent,"*** is added to the cotton to give it a bit of texture.

The shift away from petroleum-based oils and waxes has spurred the development of esters that mimic their properties. Esters can knock down foam, chase away static, build or reduce viscosity. They can cloud, opacify or even pearlize your formulation. They can be used to modify melting points, "skin feel" or other properties in a formulation.

If you want to form a protective barrier, an ester can do it. If you want to keep moisture from leaving the skin or any other substrate, an ester can do it. An ester-based massage oil is quite luxurious (or would that fall under lubricants and fragrances?)

What are esters good for? Imagine your world without them!

Chapter 4
Specialty Esters

Glycerine has been known to be a versatile raw material (bioderived-green) for its further derivatization into esters and also into its own polymeric form Polyglycerols of various degrees of polymerization. These Polyglycerols are further used to synthesize fatty acid esters of variable molecular weights and configurations. A vast number of products can be made to achieve different effects of functionalities such as emollients or emulsifiers or dispersants. Mention must be made of the following versatile materials being used in the cosmetics and personal care product industry.

1. PELEMOL 6GPR (INCI: Polyglyceryl-6 Polyricinoleate)
2. PELEMOL P-1263 (INCI: Polyglyceryl-10 Hexaoleate (and) Polyglyceryl-6 Polyricinoleate)
3. PELEMOL 10GHO (INCI: Polyglyceryl-10 Hexaoleate)
4. PELEMOL 3G22 (Polyglyceryl-3 Behenate)

These Pelemol Esters are polymeric in nature and are derived from vegetable origin sources and have become essentially favorite and versatile ingredients for the formulators. Therefore, it is felt necessary to provide more detailed technical information/data on these Technical Data Sheets. The respective Phoenomenons (i.e. TDS's) are depicted below:

PELEMOL® 6GPR

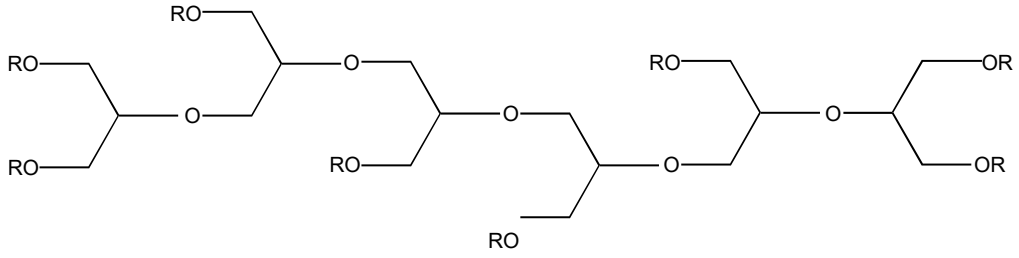
(INCI: Polyglyceryl-6 Polyricinoleate)

PELEMOL 6GPR is a 100% active, liquid, completely vegetable derived, polyester. It is very substantive to skin, lubricious, and glossy. **PELEMOL 6GPR** also exhibits considerable cushion and spreadability.

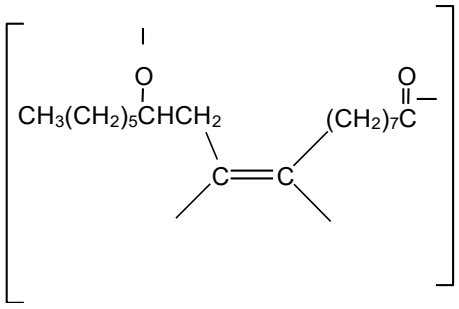
PELEMOL 6GPR contains a castor oil moiety, ricinoleic acid. Since castor oil is composed of about 80% glyceryl ricinoleate, it is not surprising that **PELEMOL 6GPR**, polyglyceryl-6 polyricinoleate, functions as a pigment wetting and dispersing agent.

These properties suggest that **PELEMOL 6GPR** would be useful as a pigment wetting and grinding aid for lipstick products and for use in skin and make-up products.

PELEMOL 6GPR is structurally described as::



Where R=

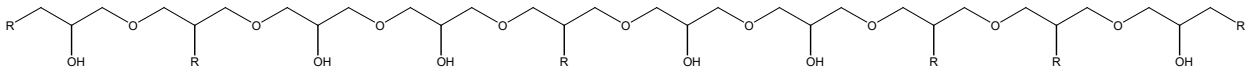


PELEMOL® 10GHO

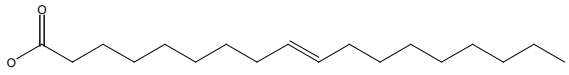
(INCI: Polyglyceryl-10 Hexaoleate)

PELEMOL 10GHO is the hexaester of Oleic Acid and Polyglyceryl-10. It is 100% active liquid and 100% vegetable derived. **PELEMOL 10GHO** is useful to deliver water dispersible lake pigments to the oil phase in lipsticks, make-up products, and eye shadows, for example. It contributes to shine and is water resistant. These properties make it useful in hair products such as leave-on conditioners. **PELEMOL 10GHO** also find application as an inorganic pigment dispersant when added to a sunscreen oil phase.

PELEMOL 10GHO is structurally described as:



where R =



Idealized structure showing R randomly distributed along linearized polyglycerin.

Trade Name:	**PELEMOL 10GHO**
INCI:	Polyglyceryl-10 Hexaoleate
CAS No:	65573-03-7

TYPICAL PROPERTIES

Appearance @ 25°C	Amber, Viscous Liquid
Color, Gardner	5
Acid Value, mg KOH/gram	2
Saponification Value, mg KOH/g	150
Moisture, kF%	1.0
Refractive Index @ 25°C	1.4695

PELEMOL® P-1263

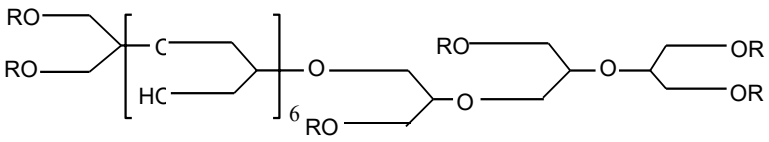
(INCI: Polyglyceryl-10 Hexaoleate (and)
Polyglyceryl-6 Polyricinoleate)

PELEMOL P-1263 is a versatile polymeric water-in-oil emulsifier for creams and lotions. **PELEMOL P-1263** is 100% active, easy to handle liquid, all vegetable derived polyester.

PELEMOL P-1263 structurally has many free hydroxyl groups on the molecules to provide considerable hydrophilic functionality and the long chain oleic and ricinoleic moieties toprovide balanced hydrophobicity.

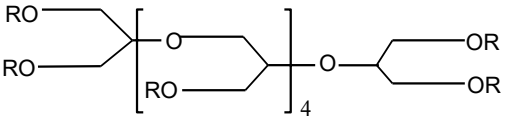
PELEMOL P-1263 with such a carefully selected structure balanced combination offers an excellent alkylene-oxide free water-in-oil emulsifier.

PELEMOL P-1263 conforms to the following blended-structure:

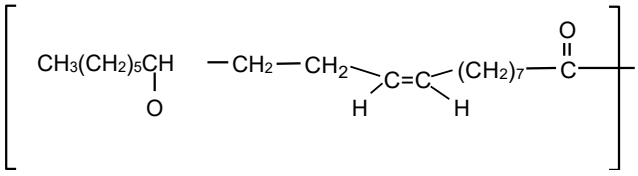


Where R= $CH_3(CH_2)_7CH=CH(CH_2)_7C(=O)-$

and



Where R =



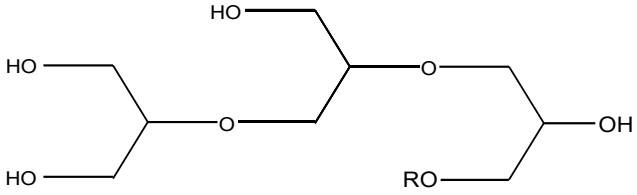
PELEMOL® 3G22

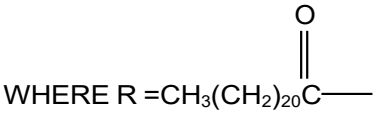
(INCI: Polyglyceryl-3 Behenate)

PELEMOL 3G22 is a 100% active, solid, all vegetable derived monoester of behenic acid and Polyglycerin-3. As such, each molecule contains four unreacted, free hydroxyl groups at one end and one long C_{22} alkyl moiety as a behenate ester at the other end.

The four free hydroxyl groups provide considerable hydrophilicity and the long behenyl alkyl hydrophobic chain enables the molecule to function as a non-alkylene oxide emulsion stabilizer.

PELEMOL 3G22 is structurally described as:





TRADE NAME	**PELEMOL 3G22**
INCI	Polyglyceryl-3 Behenate
CAS #	1207543-50-7

TYPICAL PROPERTIES

Appearance @ 25°C	Off-white Flake
Acid Value, mg KOH/gm.	3
Sap. Value, mg KOH/gm	130
Melting Point °C	74

Estolides are dimeric, trimeric, tetrameric or oligomeric esters formed by the esterification of hydroxyl fatty acid with the same or another hydroxyl containing fatty acid with elimination of water of reaction. The ester so formed is a secondary ester by nature and is relatively more resistant to aqueous hydrolysis.

The commonly used Hydroxy Fatty Acids are obtained from Castor Oil (CO) as Ricinoleic Acid (RA) also known as 12-hydroxy Oleic Acid. The variant of this is 12-hydroxy Stearic Acid (12-HSA) obtained from the Hydrogenated Castor Oil (HCO) and its subsequent hydrolysis.

The degree of esterification in this class is measured by Estolide Number (EN). The value of EN is one when two molecules of RA or HSA react to give a Dimeric Estolide. The value of EN is two when three molecules of RA or HSA to give a Trimeric Estolide. The value of EN is three when four molecules of RA or HSA to give Tetrameric Estolide. An oligomeric Estolide is thus formed by progressive esterification reaction of the hydroxyl of RA or HSA to give the desired oilgomer or more appropriately called a Homopolymer of RA or HSA.

The Estolide offered by Phoenix Chemical is:

PELEMOL PHS-8 (INCI: Polyhydroxystearic Acid)

The ideal chemical structure and its uses/applications are shown in our Phoenomenon for PELEMOL PHS-8.

PELEMOL® PHS-8

(INCI: Polyhydroxystearic Acid)

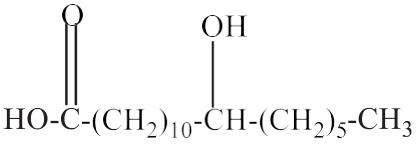
PELEMOL PHS-8 is a100% active, all vegetable derived polyester. It is a viscous,substantive, yellow liquid at ambient temperatures and as with any polymer, will tend to fractionate on cooling. Product clarity and homogeneity is restored on heating and stirring with no adverse effect on the product.

PELEMOL PHS-8 has many nucleophilic sites and, although oil soluble, will complexwater via hydrogen bonding on the skin surface. It will, therefore, function as a skin conditioner and humectant. Its substantivity and solubility profile strongly suggests its use in color cosmetics. **PELEMOL PHS-8** also functions as a superior pigment wetting, grinding, and coating agent.

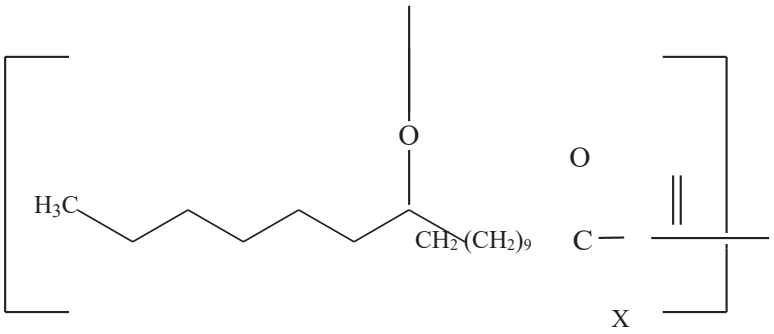
PELEMOL PHS-8 retains single terminal hydroxy and carboxy groups allowing for derivatization into many complex esters which will be the subject of patented technology.

PELEMOL PHS-8 is structurally described as**:**

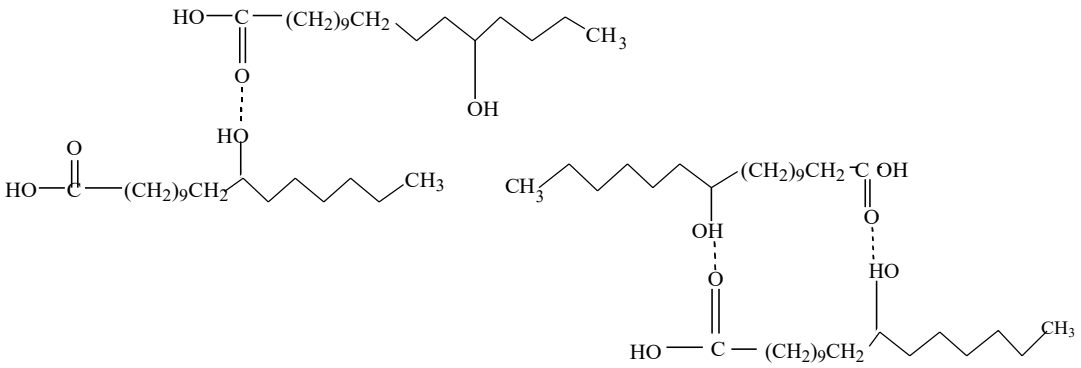
Hydroxystearic Acid



Polyhydroxystearic Acid



Gel Matrix Formation in Polyhydroxystearic Acid



PELEMOL PHS-8 (Polyhydroxystearic Acid) is a true polymeric ester; we can postulate that specific polar sites on the polymer chain will form a film in solution via hydrogen bonding with adjacent molecules to form multi-layered micelles in a polymeric liquid crystals pattern. It is this associative gel matrix formation that accounts for the superior liquid crystal emulsification properties of **PELEMOL PHS-8**.

Trade Name	**PELEMOL PHS-8**
INCI Name	Polyhydroxystearic Acid
CAS #	27924-99-8

APPLICATIONS

PELEMOL PHS-8 can be used in concentrations as much as 50% in lipsticks and its use is highly recommended in:

- Lipsticks
- Foundations
- Eye make-up
- Mascara
- Skin conditioners

TYPICAL PROPERTIES

Appearance @ 25°C	Viscous Liquid or Waxy Solid
Color (Gardner)	3
Odor	Mild, Bland
Acid Value mg KOH/gm	25
Hydroxyl Value mg KOH/gm	10
Refractive Index @ 25°C	1.4675
Specific Gravity @25°C	0.9333

*Product may separate on cooling or long-standing due to its tittering effects. Heat and stir product at 60°C to restore clarity and homogeneityat ambient temperatures before sampling and /or use. This has no adverse effects on the product.

SOLUBILITY

Water	i
Propylene Glycol	i
Ethanol	i
Mineral Oil	m
Isododecane	m
Isopropyl Myristate (Pelemol IPM)	m
Castor Oil	m
Cyclopentasiloxane(D_5)	i
Dimethicone (DC 200 Fluid, 100 cst.)	i
Isononyl Isononanoate (Pelemol IN-2)	m
Pentaerythrityl Tetraethylhexanoate (Pelemol PTO)	m

i= insoluble (at 5%)
m=miscible (soluble in all proportions)

SAFETY

* RIPT study (50 human subjects) when tested under occlusion, provides very favorable results for **PELEMOL PHS-8.**	
*Skin Irritation	NON-PRIMARY SKIN IRRITANT
*Skin Sensitization	NON-PRIMARY SKIN SENSITIZER

PELEMOL PHS-8 CAN BE DESCRIBED AS HYPOALLERGENIC

* Study conducted by AMA Labs., 216 Congers Rd. New City, NY 10956

Eye Irritation
** A HET-CAM study concluded that **PELEMOL PHS-8** has practically no ocular irritation potential.

** Study conducted by Consumer Product Testing Co., 70 New Dutch Lane,Fairfield, NJ 07004

Other Trademark Products

PHOENOXOL® Are esters of EO, PO and/or EO/PO including their isomers of $C_2 - C_{50}$ alcohols.

PHOENOXIDES® Are esters of EO, PO and/or EO/PO including their isomers of $C_2 - C_{50}$ acids.

PHOENATES®

- Phoenate GC-7 is an ester formed by the reaction of coconut acids and the polyethylene glycol ether of glycerin containing an average of 7 moles of ethylene oxide.
- Phoenate COPA is a monophosphate ester of castor oil
- Phoenate 3DSA is a stearic acid di-ester PEG-3
- Phoenate 150DSA is a stearic acid di-ester of PEG-150

Chapter 5
Analytical Methods

The following analytical methods are the most important for evaluating esters.

Method	Title
M-001	Appearance
M-002	Acid Value
M-003	Base Value
M-004	Color, Gardner
M-005	Hydroxyl Value by Acetylation
M-006	Saponification Value
M-007	Iodine Value (Wijs Method)
M-008	Titer, °C
M-009	Unsaponifiable Matter

ANALYTICAL METHOD

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M-001 -- Appearance

==========

Scope: This method is applicable to all products.

Summary: The sample is heated to the desired temperature. Once the temperature is reached, the sample is removed from the heat source and observed. A description similar to those of Table I should be reported.

Apparatus:
1. Programmable oven.
2. Steam bath.
3. Thermometer capable of reading °C and °F.

Reagents: None required.

Procedure: Loosen the cap on the sample and place the sample on a steam bath or in an oven set for the desired temperature. Remove the sample occasionally and mix well. Check the temperature of the sample using a thermometer. Once the desired temperature is reached, remove the sample from the steam bath and observe for appearance. Use Table I to assign an appearance.

Calculations: None required.

Precision:

Safety: The heated samples may cause burns. Use caution when handling.

References: None.

Table I

Appearance Classifications

Classification	Description
Sparkling Clear	No visible haze or Tyndall effect in the black box.
Clear	No visible haze in ordinary lighting, but may exhibit a Tyndall effect in the black box.
Slightly Hazy	No visible haze in ordinary lighting but visible in fluorescent lighting.
Hazy	Visible haze in ordinary lighting.

Opaque Liquid or solid through which one cannot see.

ANALYTICAL METHOD

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M-002 -- Acid Value

==========

Scope: This method is applicable to animal and vegetable fats and oils, and various products derived from them.

Summary: The acid value is the number of milligrams of potassium hydroxide necessary to neutralize fatty or rosin acids in 1 gram of sample. The sample is weighed into an Erlenmeyer flask, diluted with neutral alcohol, and titrated with 0.1N methanolic potassium hydroxide (KOH) or 0.5N aqueous sodium hydroxide (NaOH), depending on the expected acid value.

If the molecular weight of the fatty acid is known, the free fatty acid content can be calculated using the titration results.

Apparatus:
1. Erlenmeyer flasks, 250 mL.
2. Burette, 10 mL class A.
3. Burette, 50 mL class A.
4. Analytical balance, capable of determining weights to three decimal place accuracy.
5. Stir plate.
6. Stir bars.
7. Steam bath or hot plate.

Reagents:
1. Potassium hydroxide (KOH), 0.1N in methanol (Standardized using LTC-0010).
2. Sodium hydroxide (NaOH), 0.5N in water (Standardized using LTC-0020).
3. Isopropyl alcohol (IPA), reagent grade.
4. Toluene, reagent grade.
5. Chloroform, reagent grade.
6. Phenolphthalein indicator solution, 1.0% in ethanol.

Procedure:

1. Using Table I as a guide, weigh an appropriate amount of sample into a tared Erlenmeyer flask. Record the weight.

2. Add 100 mL of an appropriate neutral alcohol and a few drops of the phenolphthalein indicator solution (**Remark 1**). Place a stir bar in the flask and mix thoroughly to dissolve sample, using heat if necessary.

3. Using Table I as a guide, titrate with the appropriate solution until a faint, pink endpoint appears and persists for 30 seconds. Record the volume of titrant used to reach this endpoint and use Equation 1 in the Calculations section of this method to calculate the acid value.

4. The free fatty acid content can be calculated using Equation 2 in the Calculations section of this method.

5. The acidity (meq/gram) can be calculated using Equation 3 in the Calculations section of this method.

Calculations: Equation 1

$$\text{Acid Value, mg KOH/gram} = \frac{(\text{mL of titrant})(\text{N of titrant})(56.1)}{(\text{sample wt.})}$$

Equation 2

$$\%\ \text{Free Fatty Acid} = \frac{(\text{mL of titrant})\ (\text{N of titrant})\ (\text{Mwt. of fatty acid})}{(\text{sample wt.})\ (10)}$$

Where Mwt. lauric acid = 200
Mwt. palmitic acid = 256
Mwt. oleic acid = 282
Mwt. acetic acid = 60
Mwt. formic acid = 46

Equation 3

$$\text{Acidity, meq/gram} = \frac{(\text{mL of titrant})\ (\text{N})}{(\text{sample wt.})}$$

Precision: The relative standard deviation for acid value determinations has been determined to be ±0.5% when one sample was analyzed 36 times by different chemists on different days within the same laboratory. This relative standard deviation was determined on a sample with an average acid value of 199.8.

Based on the free fatty acid carbon chain distribution, the theoretical acid value of the sample analyzed was 199.7. Thus, this method reports 100% of the fatty acid present in the sample.

Safety: Isopropyl alcohol is flammable and a dangerous fire risk. Only handle in well ventilated areas.

Chloroform is a known carcinogen. Use in a well ventilated area. Do not get in eyes, on skin, or on clothing.

Toluene is flammable and a dangerous fire risk. Only handle in well ventilated areas.

Potassium hydroxide is corrosive. Do not get dilute solutions in eyes, on skin, or on clothing.

Sodium hydroxide is corrosive. Do not get dilute solutions in eyes, on skin, or on clothing.

Remarks: 1. A solvent system should be chosen which completely dissolves the sample and gives a sharp phenolphthalein endpoint. The three types of solvent systems which can be used are neutralized IPA, chloroform, and neutralized 50:50 IPA/toluene.

References:
1. A.O.C.S. Official Method Cd 3a-63.
2. Calgene Chemical Laboratory Notebook #501, page 71.

Table I

Sample Weight Needed to Obtain a Titration Volume Under 7 mL

Expected Acid Value	Wt. Of Sample (±10%),g	Weighing Accuracy, (± grams)	Titrating Solution
0 to 1	20	0.05	0.1N KOH
1 to 4	10	0.02	0.1N KOH
4 to 15	2.5	0.01	0.1N KOH
15 to 75	0.5	0.001	0.1N KOH
75 to 375	0.5	0.001	0.5N NaOH
375 to 1875	0.1	0.0002	0.5N NaOH

ANALYTICAL METHOD

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M-003 -- Base Value

==========

Scope: This method is applicable to all products which require a phenolphthalein endpoint such as hydroxyl value correction and assaying KOH and NaOH.

Summary: The sample is dissolved in neutralized 3A alcohol and titrated to a phenolphthalein endpoint using a dilute solution of hydrochloric acid. The results are reported internally as "Strong" base value.

Apparatus:
1. Erlenmeyer flasks, 250 mL.
2. Burette, 10 mL class A.
3. Analytical balance, capable of determining weights to three decimal place accuracy.
4. Steam bath or hot plate.
5. Stir plate.
6. Stir bars.

Reagents:
1. Hydrochloric acid (HCl), 0.1N in 3A (Standardized using LTC-0030).
2. Hydrochloric acid (HCl), 0.5N in 3A (Standardized using LTC-0030).
3. 3A alcohol absolute, 95:5:5 ethanol/methanol/IPA, reagent grade (neutralized to first phenolphthalein endpoint).
4. Phenolphthalein indicator solution, 1.0% in ethanol.

Procedure:

1. Using Table I as a guide, weigh an appropriate amount of sample into a tared Erlenmeyer flask. Record the weight.

2. Add about 75 mL of neutralized 3A alcohol and a few drops of phenolphthalein indicator solution. Place a stir bar in the flask and mix thoroughly to dissolve sample, using heat if necessary. Allow the sample solution to cool to room temperature before titrating.

3. Titrate with the appropriate HCl solution (See Table I) until the pink color disappears from the sample solution. Record the volume of titrant used to reach this endpoint. Using Equation 1 in the Calculations section of this method, determine the amine value. Report this value to one decimal place.

Calculations: Equation 1

$$(\text{mL of titrant})(\text{N of titrant})(56.1)$$

$$\text{Base Value} = \frac{\text{(sample wt.)}}{\text{(sample wt.)}}$$

Safety: The samples are basic in nature and therefore corrosive. Caution should be used when handling. Do not get in eyes, on skin, or on clothing.

Hydrochloric acid can burn skin. Do not get in eyes, on skin, or on clothing.

3A alcohol is flammable and a dangerous fire risk. Only handle in well ventilated areas.

References: 1. Hodag Method B-4.

Table I

Sample Weight Needed to Obtain a Titration Volume Under 7 mL

Expected Base Value	Wt. of Sample (+10%), g	Titrating Solution
0 to 1	20	0.1 N HCl
1 to 4	10	0.1 N HCl
4 to 15	2.5	0.1 N HCl
15 to 75	0.5	0.1 N HCl
75 to 375	0.5	0.5 N HCl
375 to 1875	0.1	0.5 N HCl

ANALYTICAL METHOD

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M-004 -- Color, Gardner

==========

Scope: This method is applicable to products in the liquid or solid state which do not differ in hue appreciably from the standards.

Summary: This method will assign a number, between 1- and 18+, which corresponds to the color of the sample as compared to a set of 18 standards. A Gardner Color may be reported on a product which differs in hue from the standards. This color will be reported as the resulting color plus the designation "Off Hue".

Apparatus:
1. 18 glass standards, 1963 series.
2. Gardner-Delta Color Comparator.
3. Comparison tubes.
4. Funnel.
5. Filter paper, Ahlstrom #505.
6. Ring stand.

Reagents: None required.

Procedure: 1. Melt the sample if it is not in a liquid state. Inspect the sample for any foreign matter and filter the sample if any is present.

2. Mix the sample thoroughly and pour into a comparison tube. Place the comparison tube in the comparator and compare with the standards to determine which standard is nearest in color to the sample.

3. Report the color of the sample as the number of the standard most closely matching the sample. If the sample falls between two standards, it will be reported as "+" or "-" (depending on whether it is darker or lighter than the standard it most closely resembles. Thus, between colors 5 and 6, the steps will be 5, 5+, 6-, and 6. If the color is lighter than 1, it will be reported as "1-". If the color is darker than 18, it will be reported as "18+".

Calculations: None required.

Precision: The color should not vary more than 1/3 unit from chemist to chemist. Off-hue products may vary up to 3 units.

Safety: The molten product is hot and may cause thermal burns. Use caution when handling.

ANALYTICAL METHOD

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M-005 -- Hydroxyl Value by Acetylation

==========

Scope: This method is applicable to any nonionic product which has primary hydroxyl values.

Summary: The hydroxyl value is the number of milligrams of potassium hydroxide equivalent to the hydroxyl content of one gram of sample. The sample is weighed into an Erlenmeyer flask and diluted with 20 mL of acetylating reagent. This mixture is refluxed for 30 minutes and titrated to a phenolphthalein endpoint with 2.0N sodium hydroxide.

Apparatus:

1. Erlenmeyer flasks, 250 mL with ground glass joints.
2. Burette, 100 mL class A with 0.1 mL divisions.
3. Analytical balance, capable of determining weights to three decimal places.
4. Stir plate.
5. Stir bars.
6. Reflux condensers with ground glass joints.
7. Pipette, 20 mL class A volumetric.
8. Graduated cylinder, 25 mL.
9. Glass bottle, >500 mL.

Reagents:

1. Sodium hydroxide (NaOH), 2.0N (Standardized using LTC-0010).
2. Pyridine, reagent grade.
3. Acetic anhydride, reagent grade.
4. Phenolphthalein indicator solution, 1.0% in ethanol.

Procedure:

Preparation of Acetylating Reagent:

1. In a glass bottle, add 1.4 mL deionized water and 400 mL pyridine. Mix thoroughly.

2. Add 50 mL acetic anhydride to the solution and mix thoroughly again.

Hydroxyl Value Analysis:

1. Every sample should be analyzed in duplicate. Use Equation 1 in the Calculations section of this method to determine the appropriate sample size (**Remark 1**). Weigh this calculated amount into a tared Erlenmeyer flask. Record the weight.

2. Pipette 20 mL of the acetylating reagent into each of the flasks containing sample as well as two Erlenmeyer flasks which will act as blanks. Add boiling stones to the samples and blanks.

3. Place all of the flasks on hot plates and connect to reflux condensers (**Remark 2**). Reflux for 30 minutes.

4. After refluxing is complete, wash down each condenser with about 10 mL of deionized water and catch the rinsing in the respective Erlenmeyer flasks.

5. Remove the flasks from the condensers and allow them to cool.

6. Add a few drops of phenolphthalein indicator solution and a stir bar to each flask. Titrate each blank and sample with 2.0 N NaOH to a faint, pink endpoint. Record the respective titration volumes and use Equation 2 in the Calculations section of this method to determine the uncorrected hydroxyl value of each sample. The corrected hydroxyl value can be determined using Equations 3 or 4, whichever is appropriate.

7. Equations 5, 6, and 7 can be used for determining the calculated hydroxyl value, average molecular weight, and % residual alcohol.

Calculations: Equation 1

$$\text{Appropriate Sample Size} = \frac{(2.5)(2.0)(56.1)}{\text{(expected OHV)}}$$

Equation 2

$$\text{Uncorrected OHV} = \frac{(\text{mL Blank} - \text{mL Sample})(N)(56.1)}{\text{sample wt.}}$$

Where Blank = average of two blank runs

Equation 3

Corrected OHV = Uncorrected OHV + Acid Value (from LTC-1010)

Equation 4

Corrected OHV = Uncorrected OHV - Base Value (from LTC-1020)

Equation 5

$$\text{Calculated OHV} = \frac{56100}{\text{Mwt of product}} \times \#\text{ of OH groups}$$

Equation 6

$$\text{Average Mwt} = \frac{56100}{\text{OHV}} \times \#\text{ of OH groups}$$

Equation 7

$$\text{Residual Alcohol, \%} = \frac{\text{OHV}}{\text{Mwt of product}} \times 100$$

Precision: The relative standard deviation for hydroxyl value determinations has been determined to be ±1.1% when one sample was analyzed 36 times by different chemists on different days within the same laboratory. This relative standard deviation was determined on a sample with an average (uncorrected) hydroxyl value of 278.6.

The corrected hydroxyl value of this sample was 278.7 and theoretical hydroxyl value of 100% pure tridecyl alcohol is 280.5. Therefore, this method reports at least 99.3% of the hydroxyl bearing molecules present in a sample.

Safety: Pyridine is flammable and toxic. Avoid breathing in fumes. Handle in well ventilated areas at all times. Do not get in eyes, on skin, or on clothing.

Acetic anhydride can cause burns and irritate eyes. Avoid breathing in fumes. Handle in well ventilated areas at all times. Do not get in eyes, on skin, or on clothing.

Sodium hydroxide is corrosive. Do not get dilute solutions in eyes, on skin, or on clothing.

Remarks: 1. The ideal titration volume of the sample is about 3/4 the titration volume of the blank. This calculation will give these titration volumes.

2. Before condensing begins, verify that there is cold water passing through the condensers. This will aid in the condensing of the samples.

References:
1. A.O.C.S. Official Method Cd 13-60.

ANALYTICAL METHOD

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M-006 -- Saponification Value

==========

Scope: This method is applicable to all fats and oils, as well as products derived from them such as esters and fatty acids.

Summary: The saponification value is the amount of alkali necessary to saponify a definite quantity of the sample. It is expressed as the number of milligrams of potassium hydroxide (KOH) required to saponify one gram of the sample.

A sample is refluxed in 0.5N methanolic KOH for 1.5 hours and titrated using 0.5N HCl.

Apparatus:

1. Erlenmeyer flasks, 250 or 300 mL with ground glass joints.
2. Liebig condensers, with ground glass joints.
3. Pipettes, 20 mL class A volumetric.
4. Burette, 50 mL class A with 0.2 mL divisions.
5. Stir bars.
6. Stir plate.
7. Hot plate.
8. Analytical balance, capable of determining weights to three decimal place accuracy.
9. Syringes, 3 and 5 mL.
10. Graduated cylinder, 25 mL.
11. Boiling stones.

Reagents:

1. Potassium hydroxide (KOH), ethanolic 0.5N (Prepared using LTC-0010), (**Remark 1)**.
2. Hydrochloric acid (HCl), 0.5N (Standardized using LTC-0030).
3. Phenolphthalein indicator solution, 0.1% in ethanol.

Procedure:

1. Melt the sample, if not a liquid, and mix thoroughly to ensure homogeneity. Using Table 1 as a guide, weigh the appropriate amount of sample into an Erlenmeyer flask (**Remark 2**). Record the weight.

2. Pipette 50 mL of 0.5N KOH into the flask, add some boiling stones, and reflux for 1.5 hours. Make sure that there is cold water going through the condensers so as to aid in the condensing of the sample back into the Erlenmeyer flasks.

3. Prepare and run a blank simultaneously with the samples by pipetting 50 ml of 0.5N KOH into an empty flask, adding some boiling stones, and refluxing along side the samples (**Remark 1**).

4. After 1.5 hours of refluxing, rinse the inside of the condensers with about 25 mL of deionized water and catch the rinsings in the Erlenmeyer

flasks. Remove the flasks from the condensers and allow the sample solutions to cool to room temperature.

5. To each flask, add 3 to 5 drops of phenolphthalein indicator and a stir bar. Titrate, while mixing, with 0.5N HCl until the pink color just disappears. Record the respective titration volumes used to reach each endpoint.

6. Using Equation 1 in the Calculations section of this method, calculate the SAP value of the samples analyzed. Report the results to one decimal place.

7. The ester value of a product can be determined using Equation 2, if the acid value is also known.

Calculations: Equation 1

$$\text{SAP value} = \frac{(\text{mL Blank} - \text{mL Sample})(\text{N of HCl})(56.1)}{(\text{wt. of sample})}$$

Equation 2

Ester value = Saponification value – Acid value

Precision: The relative standard deviation for saponification value determinations has been determined to be ±0.5% when one sample was analyzed 36 times by different chemists on different days within the same laboratory. This relative standard deviation was determined on a sample with an average saponification value of 336.0.

Using the free fatty acid carbon chain distribution of this sample, the theoretical saponification value was determined to be 336.7. Therefore, this method reports approximately 99.8% of the theoretical saponification value.

Safety: Potassium hydroxide is corrosive and can burn skin. Do not get in eyes, on skin, or on clothes.

Hydrochloric acid can burn skin. Do not get in eyes, on skin, or on clothes.

Remarks: 1. The 1.0N KOH solution is usable for at least 3 months provided the solution is protected from carbon dioxide and blanks are determined with each analysis.

2. The flask must be completely clean and completely dry before using.

References: A.O.C.S. Official Method Cd 3c-91.

Table 1

SAP Value Expected	Sample Wt. (grams)	SAP Value Expected	Sample Wt. (grams)
0 to 59	10.0 to 12.0	180 to 199	3.3 to 4.1
60 to 79	9.0 to 11.0	200 to 219	3.0 to 3.7
80 to 99	7.0 to 8.6	220 to 239	2.7 to 3.4
100 to 119	5.7 to 7.0	240 to 259	2.5 to 3.1
120 to 139	4.9 to 5.9	260 to 279	2.2 to 2.7
140 to 159	4.2 to 5.1	280 to 300	2.2 to 2.7
160 to 179	3.9 to 4.8		

ANALYTICAL METHOD

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M-007-- Iodine Value (Wijs Method)

==========

Scope: This method is applicable to all normal fatty acids, oils and fatty amines which do not contain conjugated double bonds. It cannot be used for quaternary ammonium compounds.

When iodine value is determined on fatty acids containing conjugated double bonds, the result is not to be used as a value of total unsaturation, but rather a value to compare with similar systems' degree of unsaturation (**Remark 1**).

Summary: The Iodine Value is a measure of the unsaturation of fatty acids and is expressed in terms of the number of centigrams of iodine absorbed per gram of sample (percent iodine absorbed).

A sample is dissolved in chloroform and then reacted, in the dark, with Wijs solution for a set amount of time. KI and deionized water are added to the flask and the solution is titrated with 0.1N sodium thiosulfate.

Apparatus:

1. Erlenmeyer flasks, 250 mL Iodine Determination with ground glass stoppers.
2. Analytical balance, capable of determining weights to four decimal places.
3. Pipette, 10 & 25 mL class A volumetric.
4. Burette, 50 mL class A with 0.2 mL divisions.
5. Graduated cylinders, 50 mL.
6. Stir bars.
7. Stir plate.
8. Steam bath.

Reagents:

1. Chloroform, reagent grade.
2. Wijs solution, reagent grade (**Remark 2**).
3. Potassium iodide (KI) solution, 15% in deionized water.
4. Mercuric acetate solution, 2.5% in acetic acid.
5. Sodium thiosulfate, 0.1N (Standardized using LTC-0050).
6. Starch indicator solution, 1% in deionized water (**Remark 3**).

Procedure:

1. Using Table I as a guide, weigh an appropriate amount of sample into a tared Erlenmeyer flask (**Remarks 4 & 5**). Record the weight. Label the flask accordingly.

2. Dissolve the sample by adding 25 mL of chloroform to the flask and swirling the flask. If needed, heat the flask on a steam bath to completely dissolve the sample.

3. After the sample solution has cooled to room temperature, pipette 25 mL of Wijs solution into the flask and swirl the contents till thoroughly mixed (**Remark 2 & 6**).

4. Prepare a blank sample by pipetting 25 mL of chloroform and 25 mL of Wijs solution into an empty Erlenmeyer flask (**Remark 4**). Label the flask accordingly.

5. Stopper the flasks with a ground glass stopper. Pipette about 5 mL of the 15% KI solution into the stopper well.

6. Using a timer, store the flasks in a dark place for 30 minutes (60 minutes for expected iodine values greater than 150) to allow the reaction to take place completely (**Remark 7**).

7. After the reaction is complete, remove all of the flasks from the dark at the same time. Add about 20 mL of the 15% KI solution and 75 mL of deionized water to each of the flasks. Add a stir bar to each flask and mix well.

8. Using 0.1N sodium thiosulfate, titrate the blank sample to a pale yellow endpoint (**Remark 8**). Add about 2 mL of the starch indicator solution to the flask and continue titrating until the blue color just disappears (usually a white endpoint). Repeat this titration for each of the samples.

9. Using Equation 1 in the Calculations section of this method, calculate the iodine value. Report this value to 1 decimal place.

Calculations: Equation 1

$$\text{Iodine Value (IV)} = \frac{(\text{mL Blank} - \text{mL Sample})\,(N)\,(12.69)}{\text{sample wt.}}$$

Precision: The relative standard deviation for iodine value determinations has been determined to be ±1.3% when one sample was analyzed 36 times by different chemists on different days within the same laboratory. This relative standard deviation was determined on a sample with an average iodine value of 134.7.

Safety: Chloroform is a known carcinogen. Do not breathe in vapors. Use in a well ventilated area at all times. Do not get in eyes, on skin, or on clothing.

Wijs solution causes severe burns, and the vapors can cause lung and eye damage. Use in a well ventilated area at all times. Do not get in eyes, on skin, or on clothing.

Acetic acid is corrosive and toxic. Use caution when handling. Do not get in eyes, on skin, or on clothing.

Mercuric acetate is corrosive and highly toxic. Use caution when handling. Do not get in eyes, on skin, or on clothing.

Remarks:

1. This is due to the fact that addition to one double bond of a conjugated diene and two double bonds of a conjugated triene goes rapidly but saturation of the remaining double bond is extremely slow.

2. Because the preparation of the Wijs solution is time consuming and involves the use of both hazardous and toxic chemicals, this solution may be purchased from a chemical supplier. Only use solutions which contain no carbon tetrachloride. Store in an explosion proof refrigerator to keep the solution cool and out of the light. Never allow the temperature of the solution to rise above 25-30°C. All Wijs solutions are sensitive to temperature, moisture and light.

3. The 1% starch solution can be purchased from a chemical supplier. However, if it is to be made in the lab, "Potato Starch for Iodometry" is recommended because it produces a deep blue color in the presence of the iodonium ion. "Soluble Starch" is not recommended because a consistent deep blue color may not be developed when some soluble starches interact with the iodonium ion. The following are suitable starches: Soluble Starch for Iodometry, Fisher S516-100; Soluble Potato Starch, Sigma S-2630; Soluble Potato Starch for Iodometry, J.T. Baker 4006-04.

4. All glassware must be completely clean and completely dry!

5. When analyzing dehydrated castor oil fatty acids or it's derivatives, weigh 0.11 - 0.13 grams of sample. Due to the amount of free hydroxyl groups in castor oil, it yields high iodine values.

6. When analyzing fatty amines, add 10 mL of 2.5% mercuric acetate solution along with the Wijs solution. Add 10 mL of this solution to the blank as well. The reaction time is only 3 minutes for fatty amines.

7. If the reaction is not terminated within 3 minutes of the designated reaction time (30 or 60 minutes), the sample must be discarded and reanalyzed.

8. The samples must be titrated within 30 minutes of the reaction completion (when they were removed from the dark). Otherwise, the samples must be discarded and reanalyzed.

References:

1. A.O.C.S. Official Method Cd 1-25.
2. A.O.C.S. Official Method Tg 1a-64.
3. A.O.C.S. Official Method Tg 2a-64.

ANALYTICAL METHOD

M-008-- Titer, °C

Scope: This method is applicable to fatty acids.

Summary: This method determines the solidification point or "titer" of fatty acids.

Apparatus: 1. Titer stirring assembly consisting of:
   a. Water bath (2000 mL beaker).
   b. Wide mouth bottle.
   c. Test tube, 25x100 mm.
   d. Thermometer.
   e. Wire stirrer with one end bent into a loop.
   f. Corks, six.

Reagents: None required.

Procedure: 1. Add water to the designated level of the bath.

2. Adjust water bath temperature to 15-20°C below the expected titer point.

3. Melt sample (if solid) not greater than ~15°C above expected titer.

4. Pour the sample into the test tube to be immersion mark of the thermometer.

5. Place the thermometer and wire stirrer into the test tube keeping them equidistant from the sides.

6. Place test tube assembly into wide mouth bottle.

7. The agitation with the wire stirrer is started while the temperature of sample is 10°C above the titer point.

8. Stir sample at a rate of 20 strokes per minute.

9. Record temperature of sample every minute.

10. Stir until the temperature remains constant for 30 seconds or it begins to rise.

11. Discontinue stirring immediately. Observe and record the increase in temperature.

12. The titer point is the highest temp reached by the thermometer during this rise.

Calculations: None required.
Precision: Not determined

ANALYTICAL METHOD

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M-009 -- Unsaponifiable Matter

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Scope: This method is applicable to products containing mineral oil, wax, or fatty alcohol.

Summary: This method determines the amount of matter soluble in fats and oils which cannot be saponified by caustic alkali.

Apparatus:

1. Erlenmeyer flask w/ ground glass joint, 250 mL.
2. Hot plate.
3. Condenser with cold water running through.
4. Separatory funnel, 250 mL.
5. Stokes flask w/ stopper and tubing, 250 mL.
6. Analytical balance, capable of measuring to three decimal place accuracy.
7. Dessicator capable of maintaining moisture-free environment.
8. Forced air oven capable of maintaining 105°C temperature.
9. Thermometer capable of measuring 105°C temperature.
10. Pipette bulb.
11. Pipette, 50 mL class A.

Reagents:

1. Reagent alcohol, ACS reagent grade diluted to 10% with deionized water.
2. Saponification reagent, prepared using LTC-1150.
3. Petroleum ether, ACS reagent grade.

Procedure:

1. Weigh five grams of sample into a 250 mL Erlenmeyer flask with ground glass joint. Record the weight to three decimal places.

2. Pipette 50 mL of saponification reagent into the flask.

3. Place the flask on a hot plate and connect a condenser to it with cold water running through it. Allow the solution to reflux for one hour.

4. After one hour, quantitatively rinse the inside of the condenser with about 20 mL of deionized water.

5. Remove the flask from the hot plate and quantitatively transfer the solution to a stokes flask using deionized water.

6. Add enough water to the stokes flask to bring the fluid level to the neck of the flask (just below the bulb of the flask).

7. Add about 50 mL of petroleum ether to the stokes flask. Stopper the flask and shake gently for one minute.

8. Using the stopper and glass tubing assembly, transfer the petroleum ether layer to a 500 mL separatory funnel.

9. Repeat Steps 7 and 8 until a total of five extractions are performed. Keep adding the petroleum ether layer to the same separatory funnel.

10. Add about 25 mL of the 10% reagent alcohol solution to the separatory funnel. Stopper the separatory funnel and shake gently for one minute.

11. Dispose of the 10% reagent alcohol layer.

12. Repeat Steps 10 and 11 until a total of three washes are performed of the petroleum ether layer.

13. Transfer the washed petroleum ether layer to a tared 250 mL beaker. Place the beaker on a steam bath and evaporate the petroleum ether to dryness.

14. Place the beaker in a 105°C oven for approximately 10 minutes (or until a constant weight is achieved).

15. Weigh the beaker and determine the weight of the residue to three decimal place accuracy.

16. Using Equation 1 in the Calculations section of this method, calculate the percent unsaponifiable matter in the sample. Report the results to two decimal place accuracy.

Calculations: Equation 1

$$\% \text{ Unsaponifiable Matter} = \frac{\text{Wt. of residue}}{\text{Sample wt.}} \times 100$$

Precision:

Safety: Petroleum ether is extremely flammable. Use in a well ventilated area and keep ignition sources away.

Reagent alcohol is flammable and a dangerous fire risk. Only handle in well ventilated areas.

Saponification reagent is corrosive. Do not get in eyes, on skin, or on clothing.

Methanol is flammable and toxic. Use in well ventilated areas and avoid getting in eyes, on skin, or on clothing.

Remarks:

References: 1. A.O.C.S. Official Method Tk 1a-64, reapproved 1989.

Chapter 6

Pelemol Esters

PELEMOL® EMOLLIENT ESTERS

Listed below and on the accompanying pages are PELEMOL esters having CAS, EINECS or Japanese ingredient codes.

PELEMOL® ESTERS	INCI Name	CAS No.	EINECS No.	Japanese Code No.
PELEMOL BB	Behenyl Behenate	17671-27-1	241-646-5	N/A
PELEMOL BIP	Butyphthalimide & Isopropylphthalimide	1515-72-6 304-17-6	216-157-5 206-150-5	N/A
PELEMOL BIS	Behenyl Isostearate	121877-46-1	N/A	N/A
PELEMOL C-150	Bis-Trioctyldodecyl Dilinoleate Citrate	220716-32-5	N/A	N/A
PELEMOL CA	Cetyl Acetate	629-70-9	211-103-7	510035
PELEMOL CCT	Caprylic/Capric Triglyceride	65381-09-1 73398-61-5	265-724-3 277-452-2	111164
PELEMOL CL	Cetyl Lactate	35274-05-6	252-478-7	101322
PELEMOL CP	Cetyl Palmitate	540-10-3	208-736-6	101323
PELEMOL CR	Cetyl Ricinoleate	10401-55-5	233-864-4	501146
PELEMOL DES	Diethyl Sebacate	110-40-7	203-764-5	110241
PELEMOL DIA	Diisopropyl Adipate	6938-94-9	230-072-0	101861
PELEMOL DIBA	Diisobutyl Adipate	141-04-8	205-450-3	110681
PELEMOL DICA	Diisocetyl Adipate	57533-90-1	260-799-9	512001
PELEMOL DIPS	Diisopropyl Sebacate	7491-02-3	231-306-4	110240

PELEMOL DISM	Diisostearyl Malate	67763-18-2	267-041-6	502172
PELEMOL DNPA	Dipropyl Adipate	106-19-4	203-371-9	N/A

PELEMOL® ESTERS	**INCI Name**	**CAS No.**	**EINECS No.**	**Japanese Code No.**
PELEMOL DP-72	Dipentaerythrityl Tetrahydroxystearate/Isostearate	220716-33-6	N/A	508055
PELEMOL DO	Decyl Oleate	3687-46-5	222-981-6	101696
PELEMOL DOA	Dioctyl Adipate	103-23-1	203-090-1	101915
PELEMOL DOM	Dioctyl Maleate	2915-53-9	220-835-6	523232
PELEMOL DOS	Dioctyl Sebacate	122-62-3	204-558-8	503090
PELEMOL EE	Octyldodecyl Erucate	88103-59-7	N/A	520172
PELEMOL G7A	Glycereth-7 Triacetate	57569-76-3	N/A	N/A
PELEMOL G7B	Glycereth-7 Benzoate	139247-28-2	N/A	N/A
PELEMOL G45L	Glycereth-5 Lactate	158483-23-9	N/A	N/A
PELEMOL GDLA	Glyceryl Dilaurate	27638-00-2	248-586-9	523127
PELEMOL GMB	Glyceryl Behenate	30233-64-8	250-097-0	505150
PELEMOL GMLA	Glycerel Laurate	142-18-7	205-526-6	505185
PELEMOL GMR	Glyceryl Ricinoleate	141-08-2	205-455-0	503170
PELEMOL GMU	Glycerel Undecylenate	123759-97-7	N/A	N/A
PELEMOL GTB	Tribehenin	18641-57-1	242-471-7	505124
PELEMOL GTIS	Triisostearin	26942-95-0	248-122-5	505112
PELEMOL GTL	Trilactin	537-32-6	208-664-5	N/A
PELEMOL GTO	Trioctanoin	7360-38-5	230-896-0	520818
PELEMOL HAB	Dihydroabietyl	127036-29-7	N/A	N/A

	Behenate			
PELEMOL IBS	Isobutyl Stearate	646-13-9	211-466-1	N/A
PELEMOL ICB	Isocetyl Behenate	94247-28-6	304-205-9	N/A
PELEMOL ICIS	Isocetyl Isostearate	52006-45-8	257-598-3	N/A
PELEMOL ICLA	Isocetyl Laurate	89527-28-6	N/A	N/A
PELEMOL ICO	Isocetyl Ethyl Hexanoate	125804-19-5	N/A	N/A
PELEMOL ICS	Isocetyl Stearate	25339-09-7	246-868-6	501077

PELEMOL® ESTERS	**INCI Name**	**CAS No.**	**EINECS No.**	**Japanese Code No.**
PELEMOL IDO	Isodecyl Oleate	59231-34-4	261-673-6	503028
PELEMOL IN-2	Isononyl Isononanoate	59219-71-5	261-665-2	503013
PELEMOL IPM	Isopropyl Myristate	110-27-0	203-751-4	009100
PELEMOL ISB	Isostearyl Behenate	125804-16-2	N/A	N/A
PELEMOL ISHS	Isostearyl Hydroxystearate	162888-05-3	N/A	N/A
PELEMOL ISL	Isostearyl Lactate	42131-28-2	255-674-0	N/A
PELEMOL ISNP	Isostearyl Neopentanoate	58958-60-4	261-521-9	504306
PELEMOL I-1816	Isostearyl Palmitate	72576-80-8	276-719-0	503110
PELEMOL LB	Lauryl Behenate	42233-07-8	N/A	N/A
PELEMOL LIL	Linoleyl Lactate	198133-45-8	N/A	N/A
PELEMOL LL	Lauryl Lactate	6283-92-7	228-504-8	503104
PELEMOL L2A	Laureth-2 Acetate	32289-26-2	N/A	523220
PELEMOL L20	Laureth-2 Ethyl Hexanoate	125804-14-0	N/A	N/A
PELEMOL MAR	Methyl Acetyl Ricinoleate	140-03-4	205-392-9	N/A
PELEMOL ML	Myristyl Lactate	1323-03-1	215-350-1	500308

PELEMOL MM	Myristyl Myristate	3234-85-3	221-787-9	104370
PELEMOL MS	Myristyl Stearate	17661-50-6	241-640-2	N/A
PELEMOL ODR	Octyldodecyl Ricinoleate	125093-27-8	N/A	521233
PELEMOL ODSS	Octyldodecyl Stearoyl Stearate	90052-75-8	289-991-0	508066
PELEMOL OE	Oleyl Erucate	17673-56-2	241-654-9	532030
PELEMOL OL	Oleyl Lactate	42175-36-0	N/A	N/A
PELEMOL OP	Octyl Palmitate	29806-73-3	249-862-1	509023 or 501107
PELEMOL OPG	Octyl Pelargonate	59587-44-9	261-819-9	510070

PELEMOL® ESTERS	**INCI Name**	**CASNo.**	**EINECS No.**	**Japanese Code No.**
PELEMOL OS	Octyl Stearate	22047-49-0	244-754-0	503075
PELEMOL PDD	Propylene Glycol Dicaprylate/Dicaprate	68583-51-7	271-516-3	507063
PELEMOL PGDP	Propylene Glycol Dipelargonate	41395-83-9	255-350-9	502079
PELEMOL PMR	Pentaerythrityl Monoricinoleate	N/A	N/A	N/A
PELEMOL PTA	Pentaerythrityl Tetraacetate	597-71-7	209-907-8	N/A
PELEMOL PTIS	Pentaerythrityl Tetraisostearate	62125-232-8	263-423-1	520782
PELEMOL PTL	Pentaerythrityl Tetralaurate	13057-50-6	235-946-5	N/A
PELEMOL PTO	Pentaerythrityl Tetra Ethyl Hexanoate	7299-99-2	230-743-8	520784
PELEMOL PTP	Pentaerythrityl Tetrapelargonate	14450-05-6	238-430-8	N/A
PELEMOL P-49	Pentaerythrityl Tetraisononanoate	93803-89-5	298-364-0	N/A

PELEMOL SB	Stearyl Behenate	24272-12-3	246-115-1	N/A
PELEMOL SPO	Cetearyl Octanoate	90411-68-0	291-445-1	508018
PELEMOL TAC-25	Tri $C_{12}C_{13}$ Alkyl Citrate	93573-19-4	297-554-0	532251
PELEMOL TDE	Tridecyl Erucate	131154-74-0	N/A	N/A
PELEMOL TDTM	Tridecyl Trimellitate	70225-05-7	223-994-7	N/A
PELEMOL TGC	Trioctyldodecyl Citrate	126121-35-5	N/A	532050
PELEMOL TIPC	Triisopropyl Citrate	1587-21-9	N/A	N/A
PELEMOL TISC	Trisostearyl Citrate	113431-54-2	N/A	N/A
PELEMOL® ESTERS	**INCI Name**	**CAS No.**	**EINECS No.**	**Japanese Code No.**
PELEMOL TMEB-35	Trimethylylethane Tribenzoate	N/A	N/A	N/A
PELEMOL TMPIS	Trimethylol Propane Triisostearate	68541-50-4	271-347-5	503098
PELEMOL TMPO	Trimethylolpropane Trihexyl Hexanoate	26086-33-9	N/A	503099
PELEMOL TOC	Trioleyl Citrate	175831-77-3	N/A	N/A
PELEMOL TOTM	Trioctyl Trimellitate	3319-31-1	N/A	N/A
PELEMOL 88	Ethyl Hexyl Ethyl Hexanoate	7425-14-1	231-057	N/A
PELEMOL 89	Efthyl Hexyl Isononanoate	71566-49-9	275-637-2	504050
PELEMOL 108	Isodecyl Ethyl Hexanoate	8933-26-6	N/A	N/A
PELEMOL 168	Cetyl Ethyl Hexanoate	59130-69-7	261-619-1	520159
PELEMOL 187	Stearyl Heptanoate	66009-41-4	266-065-4	504328
PELEMOL 188	Stearyl Ethyl Hexanoate	59130-7-0	261-620-7	504085
PELEMOL 300 B	C_{20-40} Alkyl Behenate	136097-81-9	N/A	N/A
PELEMOL 1215 L	C_{12-15} Alkyl Lactate	93925-36-1	300-338-1	N/A

PELEMOL 2014	Octyldodecyl Myristate	83826-43-1 22766-83-2	245-205-8	100124
PELEMOL 2022	Octyldodecyl Behenate	12804-08-2	N/A	N/A

PELEMOL® TGC

PELEMOL® TGC is a clear, oil-soluble, slightly yellow, slightly viscous triester. It is, in fact, surprisingly low in odor for a citrate triester. It is substantive to skin and extremely emollient. The hydroxyl functionality in PELEMOL® TGC makes it a uniquely effective wetting agent for pigments. In addition to its compatibility with castor oil, PELEMOL® TGC is a very effective pigment wetting and grinding vehicle for anhydrous pigment systems containing mineral oil, petrolatum, and/or microcrystalline wax due to PELEMOL® TGC's compatibility with hydrocarbons.

PELEMOL® TGC also has the unique property of being miscible with cyclomethicone, the resulting solution being extremely "silky" and soft in feel.

TRADE NAME: PELEMOL® TGC
INCI: Trioctyldodecyl Citrate
CAS #: 126121-35-5
JAPANESE CODE #: 532050

SPECIFICATIONS

Chemical Name	Trioctyldodecyl Citrate
Appearance @25°C	Clear to Hazy Oily Liquid
Color (gardner)	3 Maximum
Acid Value	5 Maximum
Sap. Value	135 – 165

SOLUBILITY

Castor Oil	m
Ethanol	i
Volatile Silicone	m
Mineral Oil	m
Propylene Glycol	i
Isopropyl Myristate	m
Water	i

m = Miscible
(Soluble @ all proportions)

i = Insoluble

APPLICATIONS

PELEMOL® TGC is useful in skin preparations where cushion is desired and is silicone compatible for such end products as creams & lotions, make-up products, lipstick & lip products, and hair products (conditioners, oils, & gels).

SAFETY

PELEMOL® TGC in an extremely safe ester. Toxicity studies are summarized as follows:

1) Primary Eye Irritation	-NON-IRRITATING
2) Primary skin Irritation	-NON-IRRITATING
3) Acute Oral Toxicity	-NON-TOXIC

PELEMOL® OE
INCI: Oleyl Erucate

The use of natural, vegetable-derived ingredients is extremely popular in modern personal care formulations. Jojoba oil is an example of such an ingredient. Availability of jojoba, like many naturally-derived materials, can vary and is subject to variations in meteorological, and seasonal conditions. PELEMOL® OE is a synthetic, vegetable-based jojoba oil substitute. This ester's physical as well as functional properties are virtually identical to jojoba oil. PELEMOL® OE can be used as a total replacement for jojoba or can be used as an economical dilutent or supplement to jojoba oil and still retain functionality and marketing claims.

PELEMOL® OE is a superb, light emollient having good dry-down and spreading characteristics. It leaves a non-oily, silky, smooth feel on the skin or hair. Its' light emolliency makes PELEMOL® OE a good choice for use in hair care products to promote shine and luster.

Recommended use levels: 1 – 10%

INCI NAME: Oleyl Erucate
CAS #: 17673-56-2
EINECS #: 241-654-9
Japanese Ingredient Code: 532030

SPECIFICATIONS

Appearance @ 25°C	Clear Liquid
Odor	Waxy
Color, Gardner	3 Max.
Hydroxyl Value	10 Max.
Acid Value, mg KOH/gram	2.0 Max.
Moisture %	0.5 Max.

SOLUBILITY

Castor Oil	m	Propylene Glycol	d	m = miscible
Ethanol	i	Isopropyl Myristate	m	(soluble @ all proportions)
Volatile Silicone	m	Water	i	d = dispersible
Mineral Oil	m			i = insoluble

PELEMOL ODSS
Octyldodecyl Stearoyl Stearate

PELEMOL® ODSS is a 100%, light, extremely emollient ester with excellent skin spreadability. It's spreadability characteristics result in a luxurious skin after-feel, with a noticeably pleasant cushion. PELEMOL® ODSS's broad oil and silicone solubility makes it an ester of choice to enhance compatibility or feel-characteristics of oil/silicone based systems. It is useful in creams and lotions at 2 – 10% levels.

INCI: Octyldodecyl Stearoyl Stearate
CAS Number: 90052-75-8
EINECS Number: 289-991-0
Japanese Ingredient Code: 508066

SPECIFICATIONS:

Appearance @ 25ºC	Clear to slightly hazy liquid
Color (Gardner)	5 Max.
Odor	Mild, characteristic
Acid Value	10 Max.
Saponification Value	115 – 135
Refractive Index	1.4550 – 1.4600
Specific Gravity	0.875 ± 0.01

SOLUBILITY:

Castor Oil	M
Ethanol	I
Volatile Silicone	M
Mineral Oil	M
Propylene Glycol	I
Isopropyl Myristate	M
Water	I

M = Miscible (soluble in all proportions)
I = Insoluble

PELEMOL® I-1816

INCI: Isostearyl Palmitate

PELEMOL® I-1816 is an all vegetable-derived, clear, practically odor-free liquid ester. It has excellent esthetic properties, producing non-greasy, tack free films. PELEMOL I-1816 exhibits good spreadability, promotes slip and has a pleasant, persistent, silky after-feel. It is recommended for incorporation into creams, lotions, lip products and stick products.

INCI Name: Isostearyl Palmitate
CAS Number: 72576-80-8
EINECS Number: 276-719-0
Japanese Ingredient Code: 503110

SPECIFICATIONS:

Appearance @ 25° C	Clear Liquid
Color (Gardner)	1.0 Max
Acid Value mg KOH/gram	2.0 Max
Odor	Slight, Typical
Saponification Value	100-115

SOLUBILITY:

Castor Oil	M
Ethanol	I
Volatile Silicone	M
Mineral Oil	M
Propylene Glycol	I
Isopropyl Palmitate	M
Water	I

M = Miscible (soluble at all proportions)
I = Insoluble

PELEMOL® IN-2
INCI: Isononyl Isononanoate

PELEMOL® IN-2 is a lightweight emollient ester with excellent spreadability. As a skin conditioner it imparts a dry, non-oily smooth after-feel to the skin. PELEMOL® IN-2 promotes slip and also helps to improve the esthetic characteristics of creams and lotions by modifying the feel of heavier emollients and occlusives. Recommended use levels: 2 - 10%

INCI Name: Isononyl Isononanoate
CAS Number: 42131-25-9
EINECS Number: 261-665-2
Japanese Ingredient Code: 503013

SPECIFICATIONS:

Appearance @ 25° C	Clear Colorless to Pale Yellow Liquid
Color (APHA)	100 Max
	Acid Value mg KOH/gram 1.0 Max
Odor	Mild, Characteristic
Saponification Value	187 - 202

SOLUBILITY:

M = Miscible (soluble at all proportions)
I = Insoluble

Castor Oil	M
Ethanol	I
Volatile Silicone	M
Mineral Oil	M
Propylene Glycol	I
Isopropyl Myristate	M
Water	I

PELEMOL® BIP

PELEMOL® BIP is a 100% active, clear, colorless liquid eutectic mixture of N-Butylphthalimide and N-Isopropylphthalimide. Each individual product exists as a solid material; however, particular blends result in a liquid having a freezing point lower that either individual component; i.e., an eutectic mixture. It functions as an excellent solvent and is finding application as a fragrance solubilizer, sunscreen solvent (solutions of 65 gms. Oxybenzone in 100 gms. PELEMOL® BIP and 40 gms. Avobenzone in 100 gms. PELEMOL® BIP @ 25ºC are possible) and nail lacquer plasticizer. PELEMOL® BIP has a slight characteristic odor and has a satiny slip on the skin.

Absorbance studies (FIG. 1) with Avobenzone in PELEMOL BIP vs. Avobenzone in IPM have demonstrated the Avobenzone in PELEMOL BIP has greater and broader absorbency than in IPM.

Trade Name: PELEMOL® BIP
INCI: Butylphthalimide Isopropylphthalimide
CAS Numbers: 1515-72-6 (N-Butylphthalimide)
304-17-6 (N-Isopropylphthalimide)
EINECS Numbers: 216-157-5 (N-Butylphthalimide)
206-150-5 (N-Isopropylphthalimide)

SPECIFICATIONS:

Appearance	Clear Liquid
% Assay	99.5% Min.
Acid Value	1.5 Max.
Ref. Index @ 25º C	1.5445 – 1.5455
% Moisture	0.2 Max.
Color (APHA)	80 Max.

SOLUBILITY:

Castor Oil	m
Ethanol	m
Volatile Silicone	i
Mineral Oil	d
Propylene Glycol	i
Isopropyl Myristate	m
Water	i
Dimethicone	i

m = miscible (soluble in all proportions)
i = insoluble
d = dispersible

SAFETY:

An RIPT study with 50 human subjects has revealed PELEMOL BIP to be:

NON – IRRITATING

NON – SENSITIZING

The study was conducted with PELEMOL BIP at a 25% level.

PATENT STATUS: Patent #: US 6,306,373 B1 October 23, 2001
Mixed N-Butyl & Iso-propyl phthalimide compounds
As sunscreen solubilizers.

Assigned to: PHOENIX RESEARCH CORPORATION

PELEMOL® OL
(INCI: Oleyl Lactate)

PELEMOL® OL is a vegetable derived, 100% active, slightly yellow, somewhat viscous liquid at ambient temperatures. PELEMOL® OL has an initial light oily feel and is characterized by its ability to leave the skin soft, supple, and silky, with an almost powdery, waxy feel on rub-in. It is extremely emollient and is unique in its ability to simultaneously both fat and moisturize the skin. PELEMOL® OL has been found to be useful in skin products, massage oils, make-up and in hair conditioners where it imparts softness, sheen and manageability.
Recommended use levels: 2 – 10%.

Trade Name: PELEMOL® OL
INCI: Oleyl Lactate
CAS Number: 42175-36-0

SPECIFICATIONS:

Appearance @ 25° C	Clear to slightly hazy liquid
Odor	Slightly Fatty
Color (Gardner)	5 Max.
Acid Value	2.0 Max.
Saponification Value	155 – 175

SOLUBILITY:

Castor Oil	M
Ethanol	I
Volatile Silicone	M
Mineral Oil	M
Propylene Glycol	D
Isopropyl Myristate	M
Water	I

M = Miscible (soluble in all proportions)
I = Insoluble
D = Dispersible

SAFETY*:

Primary Eye Irritation	- NON-IRRITATING
Primary Skin Irritation	- NON-IRRITATING
Acute Oral Toxicity	- NON-TOXIC
Comedogenicity	- NON-COMEDOGENIC

PELEMOL® ICB
INCI: Isocetyl Behenate

PELEMOL® ICB is a 100% active, low viscosity, stable, vegetable derived, liquid ester. It is both odorless and tasteless and exhibits excellent emolliency and skin spreadability characteristics.

PELEMOL® ICB exhibits broad solubility in oils and silicone, and is useful as a melting point modifier in lipstick and make-up systems. It also imparts emolliency and sheen to lipsticks, and is suitable for anhydrous skin products or emulsion systems. Use levels of 2 – 5% are indicated in skin products and 5 – 10% in lipstick and lip products.

Trade Name: PELEMOL® ICB
INCI: Isocetyl Behenate
CAS Number: 94247-28-6
EINECS Number: 304-205-9

SPECIFICATIONS:

Appearance @ 25° C	Clear, Slightly Yellow Liquid
Odor	Bland
Color (Gardner)	4 Max.
Acid Value	3 Max.
Saponification Value	70 - 95

SOLUBILITY:

Castor Oil	M
Ethanol	I
Volatile Silicone	M
Mineral Oil	M
Propylene Glycol	I
Isopropyl Myristate	M
Water	I

M = Miscible (soluble in all proportions)
I = Insoluble

SAFETY*:

Primary Eye Irritation	- NON-IRRITATING
Primary Skin Irritation	- NON-IRRITATING
Acute Oral Toxicity	- NON-TOXIC
Comedogenicity	- NON-COMEDOGENIC

PELEMOL® DP-72

INCI: Dipentaerythrityl Tetrahydroxystearate/Tetraisostearate

PELEMOL® DP-72 is the tetraester of dipentaerythrityl and hydroxystearic acid/isostearic acid. This 100% active hydrophobic, occlusive, skin conditioning, emollient ester is similar to lanolin in feel and consistency. PELEMOL® DP-72 is a paste with excellent water-holding capacity, due to the presence of hydroxyl groups in the molecule.

These characteristics make PELEMOL® DP-72 an ideal ester for use in:

- Lipstick
- High Performance Creams and Lotions
- Mascara

Recommended use levels: 1 – 10%

INCI NAME: Dipentaerythrityl Tetrahydroxystearate/Tetraisostearate
CAS #: 220716-33-6
EINECS: Polymer Exempt
Japanese Ingredient Code: 508055

SPECIFICATIONS

Appearance @ 25°C	Yellow to Amber Paste
Odor	odorless
Acid Value	1.5 Max.
Saponification Value	155 – 180
Hydroxyl Value	155 – 185

SOLUBILITY

Castor Oil	d (w)	
Ethanol	d (w)	d = dispersible
Volatile Silicone	i	i = insoluble
Mineral Oil	d (w)	s = soluble @ 5% w/w
Propylene Glycol	i	(w) = warm
Isopropyl Myristate	d (w)	
Water	i	

PELEMOL® 6GPR

PELEMOL® 6GPR is a 100% active, liquid, completely vegetable derived, polymeric octaester. It is very substantive to skin, lubricious, and glossy. PELEMOL® 6GPR also exhibits considerable cushion and spreadability.

PELEMOL® 6GPR contains a castor oil moiety, ricinoleic acid. Since castor oil is composed of about 80% glyceryl ricinoleate, it is not surprising that PELEMOL® 6GPR, polyglyceryl-6 ricinoleate, functions as a pigment wetting and dispersing agent.

These properties suggest that PELEMOL® 6GPR would be useful as a pigment wetting and grinding aid for lipstick products and for use in skin and make-up products.

TRADE NAME: PELEMOL® 6GPR
INCI: Polyglyceryl-6 Polyricinoleate
CAS #: 107615-51-0, 29894-35-7, 114355-43-0
EINECS: Polymer exempt
Japanese Code #: 511066

SPECIFICATIONS (TENTATIVE)

Appearance @ 25°C	Viscous Liquid
Color	Yellow to Amber
Acid Value	10.0 Maximum
Sap. Value	330 – 350

SOLUBILITY

Castor Oil	
Ethanol	m = Miscible (soluble @ all proportions)
Volatile Silicone	i = Insoluble
Mineral Oil	d = Dispersible
Propylene Glycol	s = Soluble
Isopropyl Myristate	(w) = warm
Water	

PELEMOL® G7A
(INCI: GLYCERETH 7 TRIACETATE)

PELEMOL® G7A is the triester of acetic acid and glycereth 7. This clear, 100% active light yellow liquid ester produces a slightly dry, silky emollience on the skin. Two properties that make PELEMOL® G7A indispensable to the cosmetic chemist is its total water-solubility and outstanding solvency, having the ability to dissolve a variety of cosmetic esters and oils. It also functions as a coupling agent in water, solubilizing water-insoluble and marginally soluble esters. PELEMOL® G7A is also a superb solvent for sunscreen actives such as Benzophenone-3, Octyl Dimethyl PABA and Octyl Methoxycinnamate.

In addition to being a multi-purpose solvent and coupling agent, PELEMOL® G7A effectively eliminates or reduces tack in carbomer gels.

PELEMOL® G7A at 5% w/w in a carbomer-based gel helps to enhance the esthetic qualities of the formulation by reducing or entirely eliminating the tacky transitional feel on hair or skin as the system dries down.

The following is a test formula illustrating the effectiveness of PELEMOL® G7A in improving the "feel" of carbomer-based gels. For best results it is recommended that PELEMOL® G7A should be added to neutralized carbomer at temperatures below 40º C.

DETACKIFICATION OF CARBOMER GELS

		A w/PELEMOL® G7A	B w/o PELEMOL® G7A
A	Deionized Water	90.30%	90.30%
	Carbomer 940	0.80	0.80
	Potassium Sorbate	0.10	0.10
B	Deionized Water	2.00	2.00
	Triethanolamine (99%)	0.80	0.80
C	PELEMOL® G7A	5.00	------
	Glycerin	------	5.00
D	Propylene Glycol (and) Diazolidinyl Urea (and) Methylparaben (and) Propylparaben	1.00	1.00

Procedure: Disperse carbomer in phase A water. When uniform dispersion is obtained add potassium sorbate with adequate agitation. Add phase B to phase A under sweep agitation. Continue slow sweep agitation and add phase D to ABC.

TRADE NAME: PELEMOL® G7A
INCI NAME: Glycereth 7 Triacetate
CAS #: 57569-76-3

SPECIFICATIONS:

Appearance	Clear Liquid
Color (Gardner)	2 Max.
Acid Value	7 Max.
Hydroxyl Value	20.0 Max.
Moisture (%)	1 Max.
Saponification Value	305-330
Activity (%)	100%

SOLUBILITY:

Castor Oil	S	
Ethanol	M	
Volatile Silicone	I	I = Insoluble
Mineral Oil	I	M = Miscible (soluble @ all proportions)
Propylene Glycol	M	S = Soluble @ 5% w/w
Isopropyl Myristate	I	
Water	M	

SAFETY*:

Primary Eye Irritation	- NON-IRRITATING
Primary Skin Irritation	- NON-IRRITATING
Acute Oral Toxicity	- NON-TOXIC
Comedogenicity	- NEGATIVE

PELEMOL® GMB
(INCI: Glyceryl Behenate)

It is known that certain high molecular weight solid esters such as PELEMOL® BB (INCI: Behenyl Behenate), when added to the oil phase of an emulsion, add richness, body and viscosity and, probably most important of all, tend to stabilize the emulsion. PELEMOL® GMB (INCI: Glyceryl Behenate) is such an ester. PELEMOL® GMB is a 100% active solid ester melting at about 70° C. It adds emolliency to any formulation and obviously can be used as a melting point modifier. PELEMOL® GMB is formulator-friendly, possessing solubility in warm oils, silicones and esters. This can be demonstrated with blends of PELEMOL® GMB and PELEMOL® TMPIS (INCI: Trimethylolpropane Triisostearate), a 100% active liquid ester that is compatible with PELEMOL® GMB in all proportions. These blends result in emollient pastes, varying in melting point with the ratio of PELEMOL® GMB to PELEMOL® TMPIS.

Additionally, PELEMOL® GMB, having a long hydrophobic tail (C_{22}) on one end of the molecule and hydroxyl groups at the other end, can function as an ethylene oxide-free, low HLB emulsifier.

These properties make PELEMOL® GMB useful in lipsticks, make-up products, and in creams and lotions. Depending on the application, recommended use levels are 2 to 10%.

Trade Name: PELEMOL® GMB
INCI: Glyceryl Behenate
CAS Number: 30233-64-8
EINECS Number: 250-097-0
Japanese Ingredient Code: 505150

S P E C I F I C A T I O N S:

Appearance @ 25° C	Off-white to yellow Coarse powder
Color (Gardner)	4 Maximum
Acid Value	5.0 Maximum
Saponification Value	140 – 160
Moisture Content, Karl Fisher	0.5% Maximum
Iodine Value, Hanus	3.0 Maximum
Melting Point (° C)	65 - 75

S O L U B I L I T Y:

Castor Oil	m(w)	
Ethanol	i	
Volatile Silicone	m(w)	m = miscible (soluble in all proportions)
Mineral Oil	m(w)	i = insoluble
Propylene Glycol	i	d = dispersible
Isopropyl Myristate	d(w)	w = warm
Water	i	

S A F E T Y*:

Primary Eye Irritation	- NON – IRRITATING
Primary Skin Irritation	- NON – IRRITATING

PELEMOL® TMPIS
(INCI: Trimethylolpropane Triisostearate)

PELEMOL® TMPIS is a 100% active, liquid triester of Trimethylolpropane and Isostearic acid. It is unique in it's sensory and visual properties. PELEMOL® TMPIS has excellent cushion and play time; it is non-tacky, light, glossy on skin, and improves application of solid delivery systems such as lipsticks and make-up products.

PELEMOL® TMPIS also exhibits broad solubility properties, dissolving in silicone as well as esters. It forms solid systems with esters such as PELEMOL® GMB (INCI: Glyceryl Behenate) for example: PELEMOL® GMB is a solid ester melting at about 70° C. PELEMOL® GMB, when melted, can be blended with PELEMOL® TMPIS to form lubricious, homogeneous, stable systems with any degree of softness required by the formulator. Similar systems are possible with other solid esters such as PELEMOL® BB (Behenyl Behenate). Low concentrations of PELEMOL® BB, such as 5%, will form very lubricious gels melting at skin temperature.

PELEMOL® TMPIS has been found to gel in mixtures with12-hydroxy stearic acid by merely stirring the 2 components with heat until they mutually dissolve and allowing the mixture to come to ambient temperatures. While firm opaque gels are formed in ratios of 70% PELEMOL® TMPIS and 30% 12-hydroxy stearic acid, for example, virtually clear firm gels are formed in ratios of 99% PELEMOL® TMPIS and 1% 12-hydroxy stearic acid. Applications for these gels are particularly seen in lipstick and lip products.

These excellent properties make PELEMOL® TMPIS an ester of choice for use in a broad range of cosmetic products such as in lipsticks and lip products, make-ups, skin creams and lotions and massage oils.

Recommended use levels: 2 – 8%.

PELEMOL® TMPIS
INCI: Trimethylolpropane Triisostearate
CAS Number: 68541-50-4
EINECS Number: 271-347-5
Japanese Ingredient Code: 503098

S P E C I F I C A T I O N S:

Appearance @ 25° C	Clear, Viscous Liquid
Color (Gardner)	2 Maximum
Moisture Content (%)	0.5 Maximum
Acid Value	2.0 Maximum
Saponification Value	175 – 195
Iodine Value, Hanus	4.0 Maximum

S O L U B I L I T Y:

Castor Oil	m
Ethanol	i
Volatile Silicone	m
Mineral Oil	m
Dimethicone	d
Propylene Glycol	i
Isopropyl Myristate	m
Water	i

m = miscible (soluble in all proportions)
i = insoluble
d = dispersible

SAFETY*:

Primary Eye Irritation	- NON – IRRITATING
Primary Skin Irritation	- NON – IRRITATING

PELEMOL® GTO
(INCI: Triethylhexanoin)

PELEMOL® GTO is the triester formed by the reaction of 2-Ethylhexanoic Acid and Glycerin. It is generally insoluble in polar solvents such as water and ethanol and soluble in oils such as castor oil, volatile silicone and mineral oil.

PELEMOL® GTO is a light, very emollient, non-tacky ester with light cushion and spreadability. These properties and it's solubility characteristics make PELEMOL® GTO particularly useful in lipsticks and make-up products. Additionally, it's registration status make it an ideal ester for use in global products.

Recommended use levels vary from 3 to 10%.

Trade Name: PELEMOL® GTO
Chemical Name: Glyceryl Triethylhexanoate
INCI: Triethylhexanoin
CAS Number: 7360-38-5
EINECS Number: 230-896-0
Japanese Registration Number: 520818

SPECIFICATIONS:

Appearance @ 25° C	Clear Liquid
Color	Light Yellow
Odor	Typical, Mild
Acid Value	2.0 Maximum
Refractive Index @ 25° C	1.446 ± 0.009
Saponification Value	340 - 360

SOLUBILITY:

Castor Oil	m
Ethanol	i
Volatile Silicone	m
Mineral Oil	m
Propylene Glycol	d
Isopropyl Myristate	m
Water	i

m = miscible (soluble in all proportions)
i = insoluble
d = dispersible

SAFETY*:

Primary Eye Irritation	- NON – IRRITATING
Primary Skin Irritation	- NON – IRRITATING

PELEMOL® GTIS
(INCI: Triisostearin)

PELEMOL® GTIS is a 100% active, liquid triester. The reaction product of Glycerine and Isostearic acid, PELEMOL® GTIS exhibits excellent cushion and is uniquely suited for use in lipstick, lip gloss, and other lip products where it can also be useful in modifying melting points. On rub-in, PELEMOL® GTIS leaves the skin with a lubricious and glossy appearance.

PELEMOL® GTIS also exhibits broad solubility properties, dissolving in other esters, oils and silicone. These solubility properties make it very compatible and "formulator friendly"; i.e., it lends itself to being formulated with other ingredients with ease.

PELEMOL® GTIS is adaptable to "global" formulations. It's excellent spreadability and cushion also indicates it's use in skin products.

Recommended use levels: 2 – 8%.

Trade Name: PELEMOL® GTIS

INCI: Triisostearin

CAS Number: 26942-95-0

EINECS Number: 248-122-5

Japanese Ingredient Code: 505112

PELEMOL GTIS

S P E C I F I C A T I O N S;

Appearance @ 25° C	Clear Liquid
Color (Gardner)	3 Maximum
Acid Value	2.0 Maximum
Saponification Value	173 – 199

S O L U B I L I T Y:

Castor Oil	m	
Ethanol	i	
Volatile Silicone	m	m = miscible (soluble in all proportions)
Mineral Oil	m	
Propylene Glycol	i	i = insoluble
Isopropyl Myristate	m	
Water	i	

S A F E T Y*:

Primary Eye Irritation	- NON – IRRITATING
Primary Skin Irritation	- NON – IRRITATING

PELEMOL® DISM

(INCI: Diisostearyl Malate)

PELEMOL® DISM is a 100% active liquid diester of an alpha hydroxy acid. This ester exhibits excellent skin feel characterized by cushion and emolliency leaving the skin soft and supple. PELEMOL® DISM is oil and silicone soluble and can be formulated with these materials in a variety of cosmetic products.

PELEMOL® DISM is suitable for lipstick and lip products as well as make-up and skin formulations.

Recommended use levels: 2 – 10%.

Trade Name: PELEMOL® DISM

INCI: Diisostearyl Malate

CAS Number: 67763-18-2

EINECS Number: 267-041-6

Japanese Ingredient Code: 502172

SPECIFICATIONS:

Appearance @ 25°C	Clear Liquid
Color (Garner)	1 Max.
Odor	Practically Odorless
Acid Value	1.0 Max.
Saponification Value	165 – 180
Hydroxyl Value	70 – 90

SOLUBILITY:

Caster Oil	m	
Ethanol	i	
Volatile Silicone	m	m = miscible (soluble in all Proportions)
Mineral Oil	m	
Propylene Glycol	i	i = insoluble
Isopropyl Myristate	m	
Water	i	

PELEMOL® TAC-25
INCI: Tri C_{12-13} Alkyl Citrate

PELEMOL® TAC-25 is a 100% active, virtually odorless, water white triester of citric acid and C_{12-13} alcohols. It is caster oil compatible and an effective pigment wetting and dispersing agent. It can be used in place of caster oil in pigmented systems for low odor or fragrance free products.

PELEMOL® TAC-25 can be gelled with 12-hydroxystearic acid. It will form translucent gels in the 1.5 to 6% 12-hydroxystearate range. As the concentration of 12-hydroxystearic acid increases above 6% the gels become opaque rather than translucent. The most important property of these gels is their extremely luxurious feel while at the same time evidencing little to no payout.

These properties make PELEMOL® TAC-25 an ester of choice for transfer proof lipstick, lip balms, and other lip and transfer-resistant make-up products.

PELEMOL® TAC-25 can also be formulated into clear, fragrance free skin products.

Having CAS, EINECS, and Japanese registration numbers PELEMOL® TAC-25 is suitable for global cosmetic products.

Recommended use levels: 3 to 20%.

Trade Name: PELEMOL® TAC-25
INCI: Tri Alkyl C_{12-13} Citrate
CAS Number: 93573-19-4
EINECS Number: 297-554-0
Japanese Registration Number: 532251

S P E C I F I C A T I O N S:

Appearance @ 25° C	Clear oily liquid
Color (Gardner)	1 Maximum
Moisture, %	0.5 Maximum
Acid Value	5.0 Maximum
Saponification Value	205 – 235

S O L U B I L I T Y:

Caster Oil	m	
Ethyl Alcohol	i	
Volatile silicone	m	m = miscible (soluble in water in all proportions)
Mineral Oil	m	
Propylene Glycol	i	i = insoluble
IPM	m	
Water	i	

PELEMOL® LIL
INCI: Linoleyl Lactate

PELEMOL® LIL is an emollient that can be described as neither oily nor dry. It possesses a unique skin-feel that benefits a variety of personal care formulations. A member of Phoenix Chemical's line of alpha-hydroxy acid esters, this emollient not only provides moisturization through a semi-occlusive barrier effect, but also delivers the alpha-hydroxy acid *lactic acid* via a slow release owing to the skin's own natural esterases. These are enzymes found in the epidermis that can hydrolyze esters and in the case of PELEMOL® LIL, free up lactic acid so that it may perform its exfoliating effect. In its unhydrolyzed form, PELEMOL® LIL functions as an emollient and humectant, because of its ability to decrease the rate of transepidermal water loss through occlusion and its ability to bind water from the atmosphere and deeper, more hydrated layers of the epidermis through hydrogen bonding with its free hydroxyl group.

PELEMOL® LIL
Trade Name: PELEMOL® LIL
INCI: Linoleyl Lactate
CAS #: 198133-34

SOLUBILITY

Caster Oil	m	
Ethanol	i	m = Miscible
Volatile Silicone	m	i = Insoluble
Mineral Oil	m	(soluble @ all proportions)
Propylene Glycol	i	
Isopropyl Myristate	m	
Water	i	

SPECIFICATIONS

Appearance @25°C	Clear Liquid
Color	Amber
Odor	Mild
Acid Value	10 Maximum

PELEMOL® PTIS

INCI: Pentaerythrityl Tetraisostearate

PELEMOL® PTIS is a rapidly absorbed emollient. It possesses cushion and a slight amount of drag. In addition to these attributes, it has an extremely bland taste, making it particularly useful to lipstick and lip treatment formulas. For applications where shine is undesirable, PELEMOL® PTIS performs well because of its matte appearance on the skin.

It is supplied as a 100% active, clear, straw-colored liquid that is compatible with a variety of personal care raw materials. This medium viscosity emollient is a valuable addition to the palettes of both color cosmetic and skin care formulators.

PELEMOL® PTIS:

TRADE NAME: Pelemol® PTIS
INCI: Pentaerythrityl Tetraisostearate
CAS NUMBER: 62125-232-8
EINECS NUMBER: 263-423-1
JAPANESE INGREDIENT CODE: 520782

SOLUBILITY

Castor Oil	m	
Ethanol	i	m = Miscible
Volatile Silicone	m	i = Insoluble
Mineral Oil	m	(soluble @ all proportions)
Propylene Glycol	i	
Isopropyl Myristate	m	
Water	i	

SPECIFICATIONS

Appearance @25°C	Clear Liquid
Color, ASTM	2 Maximum
Moisture, %	0.1 Maximum
Acid Value	2 Maximum

SAFETY

An RIPT study with 50 human subjects has revealed PELEMOL® PTIS to be:

NON-IRRITATING
NON-SENSITIZING

PELEMOL® OE
INCI: Oleyl Erucate

The use of natural, vegetable-derived ingredients is extremely popular in modern personal care formulations. Jojoba oil is an example of such an ingredient. Availability of jojoba, like many naturally-derived materials, can vary and is subject to variations in meteorological, and seasonal conditions. PELEMOL® OE is a synthetic, vegetable-based jojoba oil substitute. This ester's physical as well as functional properties are virtually identical to jojoba oil. PELEMOL® OE can be used as a total replacement for jojoba or can be used as an economical dilutent or supplement to jojoba oil and still retain functionality and marketing claims.

PELEMOL® OE is a superb, light emollient having good dry-down and spreading characteristics. It leaves a non-oily, silky, smooth feel on the skin or hair. Its' light emolliency makes PELEMOL® OE a good choice for use in hair care products to promote shine and luster.

Recommended use levels: 1 – 10%

INCI NAME: Oleyl Erucate
CAS #: 17673-56-2
EINECS #: 241-654-9
Japanese Ingredient Code: 532030

SPECIFICATIONS

Appearance @ 25°C	Clear Liquid
Odor	Waxy
Color, Gardner	3 Max.
Hydroxyl Value	10 Max.
Acid Value, mg KOH/gram	2.0 Max.
Moisture %	0.5 Max.

SOLUBILITY

Castor Oil	m	Propylene Glycol	d	m = miscible
Ethanol	i	Isopropyl Myristate	m	(soluble @ all proportions)
Volatile Silicone	m	Water	i	d = dispersible
Mineral Oil	m			i = insoluble

PELEMOL® 6GPR

PELEMOL® 6GPR is a 100% active, liquid, completely vegetable derived, polymeric octaester. It is very substantive to skin, lubricious, and glossy. PELEMOL® 6GPR also exhibits considerable cushion and spreadability.

PELEMOL® 6GPR contains a castor oil moiety, ricinoleic acid. Since castor oil is composed of about 80% glyceryl ricinoleate, it is not surprising that PELEMOL® 6GPR, polyglyceryl-6 ricinoleate, functions as a pigment wetting and dispersing agent.

These properties suggest that PELEMOL® 6GPR would be useful as a pigment wetting and grinding aid for lipstick products and for use in skin and make-up products.

TRADE NAME: PELEMOL® 6GPR
INCI: Polyglyceryl-6 Polyricinoleate
CAS #: 107615-51-0, 29894-35-7, 114355-43-0
EINECS: Polymer exempt
Japanese Code #: 511066

SPECIFICATIONS

Appearance @ 25°C	Viscous Liquid
Color	Yellow to Amber
Acid Value	10.0 Maximum
Sap. Value	330 – 350

SOLUBILITY

Castor Oil	
Ethanol	m = Miscible (soluble @ all proportions)
Volatile Silicone	i = Insoluble
Mineral Oil	d = Dispersible
Propylene Glycol	s = Soluble
Isopropyl Myristate	(w) = warm
Water	

PELEMOL® 89

PELEMOL® 89 is a liquid, water-insoluble, low-viscosity, 100% active ester. It is extremely dry, and this non-oily skin feel frequently makes it a preferred emollient in many skin and make-up products. PELEMOL® 89 is useful in reducing tackiness in antiperspirant sticks and as a partial replacement for expensive emollients.

TRADE NAME: PELEMOL® 89
INCI: Ethylhexyl Isononanoate
CAS #: 71566-49-9
EINECS #: 275-637-2
JAPANESE CODE #: 504050

SPECIFICATIONS

Chemical Name	2-Ethylhexyl Isononanoate
Appearance @25°C	Clear, Slightly Yellow Liquid
Color (APHA)	100 Maximum
Acid Value	1.0 Maximum
Iodine Value	1.0 Maximum
Sap. Value	200 – 215

SOLUBILITY

Castor Oil	m
Ethanol	m
Volatile Silicone	m
Mineral Oil	m
Propylene Glycol	i
Isopropyl Myristate	m
Water	i

m = Miscible
(soluble @ all proportions)

i = Insoluble

APPLICATIONS

PELEMOL® 89 is a very dry emollient useful in skin preparations where dryness on rub-in is desirable such as in creams & lotions, lipsticks, antiperspirant sticks, make-up products, and nail cuticle treatments.

SAFETY

PELEMOL® 89 toxicity studies were performed with 100% product, undiluted by extenders, with very favorable results as summarized below:

1) Primary Eye Irritation - NON-IRRITATING

2) Primary skin Irritation - NON-IRRITATING

3) Acute Oral Toxicity - NON-TOXIC

4) Comedogenicity - NON-COMEDOGENIC

PELEMOL® G45L

PELEMOL® G45L is a 100% active, nonionic, emollient humectant derived from naturally occurring materials and is hygroscopic in nature. It is soluble in water, ethanol, isopropanol and insoluble in mineral oil. These solubility characteristics make it useful in hydro-alcoholic formulations. PELEMOL® G45L is useful in products where an extremely soft after-feel is desired. A member of Phoenix Chemical's line of alpha-hydroxy acid esters, this emollient not only provides moisturization through a semi-occlusive barrier effect, but also delivers the alpha-hydroxy acid *lactic acid* via a slow release owing to the skin's own natural esterases. These are enzymes found in the epidermis that can hydrolyze esters and in the case of PELEMOL® G45L, free up lactic acid so it may perform its exfoliating affect. In its unhydrolyzed form, PELEMOL® G45L functions as emollient and humectant, because of its ability to decrease the rate of transepidermal water loss through occlusion and its ability to bind water from the atmosphere and lower, more hydrated layers of the epidermis through hydrogen bonding with its free hydroxyl group.

TRADE NAME: PELEMOL® G45L
INCI: Glycereth-5 Lactate
CAS #: 12804-28-6

SPECIFICATIONS

Chemical Name	Glycereth-4.5 Lactate
Appearance @25°C	Clear Viscous Liquid
Color (APHA)	100 Maximum
Acid Value	5 Maximum
Sap. Value	150 – 170

SOLUBILITY

Castor Oil	d
Ethanol	m
Volatile Silicone	i
Mineral Oil	i
Propylene Glycol	m
Isopropyl Myristate	i
Water	m

m = Miscible
(soluble @ all proportions)

i = Insoluble

d = Dispersible

APPLICATIONS

PELEMOL® G45L is an emollient. It is the perfect coupler for hydro-alcoholic fragrance systems allowing inclusion of water while maintaining clarity. Useful in after-shave products, creams and lotions, splash-on products, and make-up products.

SAFETY

PELEMOL® G45L toxicity studies were performed with 100% product, undiluted by extenders, with very favorable results as summarized below:

1) Primary Eye Irritation - NON-IRRITATING

2) Primary skin Irritation - NON-IRRITATING

3) Acute Oral Toxicity - NON-TOXIC

4) Comedogenicity - NON-COMEDOGENIC

PELEMOL® ISL

PELEMOL® ISL is a 100% active, oil-soluble, liquid ester. It is extremely lubricious and silky to the touch and particularly designed for skin application. This alpha-hydroxy acid derivative lends moisturization and softness to the skin, and the product will enrich and enhance formulations designed for application to the body, resulting in a pleasant after-feel. A member of Phoenix Chemical's line of alpha-hydroxy acid esters, this emollient not only provides moisturization through a semi-occlusive barrier effect, but also delivers the alpha-hydroxy acid *lactic acid* via a slow release owing to the skin's own natural esterases. These are enzymes found in the epidermis that can hydrolyze esters and in the case of Pelemol® ISL, free up lactic acid so it may perform its exfoliating affect. In its unhydrolyzed form, Pelemol® ISL functions as emollient and humectant, because of its ability to decrease the rate of transepidermal water loss through occlusion and its ability to bind water from the atmosphere and lower, more hydrated layers of the epidermis through hydrogen bonding with its free hydroxyl group.

PELEMOL® ISL is also useful as a sesame oil replacement.

TRADE NAME: PELEMOL® ISL
INCI: Isostearyl Lactate
CAS #: 42131-28-2
EINECS #: 255-674-0

SPECIFICATIONS

Chemical Name	Isooctadecyl 2-Hydroxypropanoate
Appearance @ 25°C	Clear Yellow Liquid
Color (Gardner)	4 Maximum
Acid Value	5.0 Maximum
Sap. Value (mg KOH/g)	130-155

SOLUBILITY

Caster Oil	m
Ethanol	i
Volatile Silicone	m
Mineral Oil	m
Propylene Glycol	d
Isopropyl Myristate	m
Water	i

m = Miscible
(soluble @ all proportions)

i = Insoluble

d = Dispersible

APPLICATIONS

PELEMOL® ISL is suitable for use in:

1) Skin Creams and Lotions
2) Lipstick and Lip Products
3) Body Lotions
4) Bath Gels
5) Eye Shadows
6) Mascaras
7) Blushes
8) Cuticle Treatments

SAFETY

Toxicity studies have shown PELEMOL® ISL to be extremely safe; results are summarized below:

1) Primary Eye Irritation - NON-IRRITATING

2) Primary skin Irritation - NON-PRIMARY IRRITANT

PELEMOL® EE

PELEMOL® EE is an oil-soluble, 100% active, liquid ester. It is completely vegetable-derived. For a long carbon chain length ester (42 carbon atoms), it is surprisingly very low in viscosity, and has excellent shelf-life and clarity at low temperatures. It is readily absorbed into skin leaving a soft, smooth, non-greasy, dry feel. PELEMOL® EE also rapidly absorbs into leather surfaces.

TRADE NAME: PELEMOL® EE
INCI: Octyldodecyl Erucate
CAS #: 132208-25-4
JAPANESE CODE #: 520172

SPECIFICATIONS

Chemical Name	Eicosyl Erucate
Color (Gardner)	3 Maximum
Acid Value (mg KOH/g)	1.0 Maximum
Residual Alcohol (%)	1.5 Maximum
Water (%)	0.05 Maximum

SOLUBILITY

Castor Oil	m
Ethanol	i
Volatile Silicone	m
Mineral Oil	m
Propylene Glycol	i
Isopropyl Myristate	m
Water	i

m = Miscible
(soluble @ all proportions)

i = Insoluble

APPLICATIONS

PELEMOL® EE is suitable for use in:

1) Creams and Lotions
2) Make-up Products
3) Nail Cuticle Treatments
4) Antiperspirant Sticks
5) Lipstick
6) Leather Conditioning
7) Shave & After-Shave Products
8) Splash-On Products

SAFETY

Toxicity studies have shown PELEMOL® EE to be extremely safe; results are summarized below:

1) Primary Eye Irritation - NON-IRRITATING
2) Primary Skin Irritation - NON-PRIMARY IRRITANT
3) Acute Oral Toxicity - ORALLY NON-TOXIC
4) Comedogenicity - NON-COMEDOGENIC

PELEMOL® ISB

PELEMOL® ISB is a 100% active ester and exists as a soft, opaque, off-white paste at ambient temperatures. It melts at skin temperature and imparts an extremely emollient and soft feel to skin. PELEMOL® ISB is generally soluble in oil and insoluble in water. It is an effective moisture barrier and imparts “slip” to powders

TRADE NAME: PELEMOL® ISB
INCI: Isostearyl Behenate
CAS #: 125804-16-2

SPECIFICATIONS

Chemical Name	Isostearyl Behenate
Appearance @ 25°C	Soft Paste
Color	White to Off-White
Acid Value	3.0 Maximum
Sap. Value	80 - 100
Melting Point	31 - 37° C

SOLUBILITY

Castor Oil	s(w)
Ethanol	i
Volatile Silicone	s(w)
Mineral Oil	s(w)
Propylene Glycol	i
Isopropyl Myristate	m(w)
Water	i

m = Miscible
(soluble @ all proportions)

i = Insoluble

s=Soluble

(w)=Warm

APPLICATIONS

PELEMOL® ISB is silicone-compatible and is useful in lotions & creams, lipsticks, mascara, liquid eye make-up, eye shadow, stick deodorants, hair grooming products, and powder make-up.

SAFETY

PELEMOL® ISB in an extremely safe ester. Toxicity studies are summarized as follows:

1) Primary Eye Irritation - NON-IRRITATING
2) Primary skin Irritation - NON-IRRITATING
3) Acute Oral Toxicity - NON-TOXIC
4) Comedogenicity - NON-COMEDOGENIC

PELEMOL® L2A

PELEMOL® L2A is a colorless, odorless, 100% active ester. It is characterized by an extremely silky, smooth and emollient feel. PELEMOL® L2A is completely soluble in ethanol and disperses in water with a white bloom. It is a useful emollient in hydro-alcoholic systems where complete clarity is desired. It is also useful in bath preparations as a blooming agent. PELEMOL® L2A's marginal water-solubility appears to cause it to deposit on the skin when incorporated into a blooming bath oil, leaving the skin with a luxurious feel. It is also compatible in detergent systems leaving a soft feel in both skin and hair after rinse-off

TRADE NAME: PELEMOL® L2A
INCI: Laureth-2 Acetate
CAS #: 32289-26-2

SPECIFICATIONS

Chemical Name	Laureth-2 Acetate
Appearance @25°C	Clear Liquid
Color	Colorless to Pale Yellow
Acid Value	5.0 Maximum
Sap. Value	46 – 86

SOLUBILITY

Castor Oil	m
Ethanol	m
Volatile Silicone	d
Mineral Oil	s
Propylene Glycol	m
Isopropyl Myristate	m
Water	d

m = Miscible
(soluble @ all proportions)

s=Soluble

d=Dispersible

APPLICATIONS

PELEMOL® L2A is a very light and emollient ester. It is useful in bath products, body oils, massage cream, liquid hand soaps, and hair products.

SAFETY

PELEMOL® L2A in an extremely safe ester. Toxicity studies are summarized as follows:

1) Primary Eye Irritation - NON-IRRITATING

2) Primary skin Irritation - NON-IRRITATING

3) Acute Oral Toxicity - NON-TOXIC

PELEMOL® TISC
(INCI: Triisostearyl Citrate)

PELEMOL® TISC is a viscous, slightly yellow, 100% active liquid, triisostearyl ester of citric acid. Citric acid is a tetrafunctional molecule containing three carboxy and one hydroxy group. In PELEMOL® TISC, the three carboxy groups are esterfied leaving a free hydroxy group. This free hydroxy group creates a degree of hydrophylicity, facilitating emulsification and wetability. PELEMOL® TISC is soluble in most vegetable and mineral oils, esters, and Cyclomethicone. It is insoluble in water, ethanol, and glycols. PELEMOL® TISC is all vegetable derived.

Trade Name: PELEMOL® TISC
Chemical Name: Triisostearyl Citrate
INCI: Triisostearyl Citrate
CAS Number: 113431-54-2

APPLICATIONS:

PELEMOL® TISC is recommended as a pigment wetting and dispersing agent. It helps impart spreadability and gloss in lipstick and make-up products. It is a virtually odorless and tasteless product making it an ideal candidate for color cosmetics.

SPECIFICATIONS:

Appearance @ 25°C	Viscous Liquid
Color (APHA)	150 Maximum
Acid Value	2.0 Maximum
Iodine Value	3.0 Maximum
Saponification Value	150 – 165

SOLUBILITY:

Castor Oil	m
Ethanol	i
Volatile Silicone	m
Mineral Oil	m
Propylene Glycol	i
Isopropyl Myristate	m
Water	i

m = miscible (soluble in all proportions)

i = insoluble

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