(19) World Intellectual Property Organization

International Bureau





(10) International Publication Number

WO 2009/083735 A1

(43) International Publication Date

9 July 2009 (09.07.2009)

C07C 69/78 (2006.01) A61K 8/00 (2006.01) (21) International Application Number:

(51) International Patent Classification:

PCT/GB2008/051227

(22) International Filing Date:

23 December 2008 (23.12.2008)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

0725266.1

28 December 2007 (28.12.2007)

(71) Applicant (for all designated States except US): IN-NOSPEC LIMITED [GB/GB]; Innospec Manufacturing Park, Oil Sites Road, Ellesmere Port, Cheshire CH65 4EY (GB).

(72) Inventors; and

(75) Inventors/Applicants (for US only): SYED, Samad [US/US]; 126 Linwood Avenue, Paramus, New Jersey 07652 (US). COTRELL, Phillip [US/US]; 410 Wildwood Drive, Salisbury, North Carolina 28146 (US).

(74) Agent: PIDGEON, Robert, John; Appleyard Lees, 15

Clare Road, Halifax HX1 2HY (GB). (81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM,

AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH. CN. CO. CR. CU. CZ. DE. DK. DM. DO. DZ. EC. EE. EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ. TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

- with international search report
- before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments



(54) Title: NOVEL ESTERS AND COMPOSITIONS AND USES THEREOF

(57) Abstract: A novel ester of an optionally substituted aromatic acid (for example benzoic acid) and a branched C₁₃ primary alcohol is suitable for use in providing improved cosmetic and personal care compositions including sunscreen, antiperspirant and deodorant compositions.

1

NOVEL ESTERS AND COMPOSITIONS AND USES THEREOF

This invention relates to aromatic esters (for example benzoate esters) of C13 branched chain fatty alcohols, and their use in topical cosmetic compositions.

US 4,275,222 describes benzoic acid esters of a mixture of C_{12} , C_{13} , C_{14} and C_{15} primary alcohols, and their use as diluents, solvents, plasticizers and liquid carriers, notably for use in toiletry or cosmetic products, dyestuffs or textiles. It is stated that in such alcohols at least 70% by weight of the alcohol of each specific chain length is linear. The branching (if any) comprises about 50% of methyl groups with smaller amounts of ethyl, propyl, butyl, aryl and hexyl groups. The alcohols are said to be commercially available.

It has now been determined that certain esters which may be present as components within the mixtures described in US 4,275,222, when added as an emollient to a cosmetic composition, particularly a sunscreen composition, provides new and unexpected properties when compared to said mixtures.

In accordance with a first aspect of this invention there is provided an ester of an optionally substituted aromatic acid and a branched C_{13} primary alcohol.

A preferred ester is an ester of an optionally substituted benzoic acid and a branched C_{13} primary alcohol. A general formula for said preferred ester may be given as

5

10

15

20

2

$$(Q)_m$$
 Q R (I)

where Q is a substituent, as later defined; m is 0 (zero) or an integer from 1 to 5 (the groups Q being the same as or different from each other when m is 2, 3, 4 or 5); and R is a branched C_{13} alkyl group.

5

10

The benzene ring (or other aromatic ring system) may be substituted with 0 to 5 groups (in addition to the reacted acid group COOH). For example it may be tri- or di-substituted in the ring (or ring system) or, more preferably, mono-substituted. Substitution may be at the ortho, and/or meta, and/or para position(s).

The or each substituent may be any common group used for 15 substitution of a benzene ring (or other aromatic ring system), for example one or more of an alkyl group (an especially preferred substituent), an alkenyl group, a haloalkyl group, an alkynyl group, a nitrile group, a carboxylic acid (in addition to the reacted carboxylic acid group), an ester, an ether, an 20 alkoxy group, a haloalkoxy group, a halo group, a hydroxyl group, a mercapto group, an alkylmercapto group, an alkylsulfoxy group, a sulfoxy group, an aryl group, an arylalkyl group, a substituted or unsubstituted amine group or a nitro group. Within these substituents an alkyl group, including of the alkyl 25 moiety of an alkyl-containing group (for example alkoxy or haloalkyl) is suitably a C_{1-4} alkyl group, more preferably a methyl group. Alternatively, and most preferably, the benzene

ring (or other aromatic ring system) is unsubstituted (i.e. m is zero).

The branched C_{13} primary alcohol backbone may be branched at one or more positions of the backbone of the primary alcohol.

The branched C_{13} primary alcohol residue is preferably branched from one position only, of the backbone of the primary alcohol.

10 The branched C_{13} primary alcohol residue preferably contains from 1 to 6 carbon atoms, in one or more side chains.

The branched C_{13} primary alcohol residue preferably has a C_{1-6} alkyl side chain. A C_{3-6} alkyl side chain, when present, is preferably an $n-C_{3-6}$ alkyl group. However a preferred side chain is an ethyl group or, especially, a methyl group.

15

20

25

Preferably the branched C_{13} primary alcohol residue is branched from the carbon atom second furthest from the optionally substituted aromatic moiety.

An especially preferred ester of the first aspect of the present invention has the formula

$$O$$
 CH_{2}
 O
 (II)

WO 2009/083735

4

PCT/GB2008/051227

Preferably a compound of the first aspect is provided in at least 90% by weight pure form, more preferably at least 95%, and most preferably at least 98%. In an especially preferred embodiment it is provided in a substantially pure form.

5

10

15

It has been discovered that esters of the first aspect, for example compounds of formula I or II, can produce enhanced properties when added to cosmetic compositions. These enhanced properties make such compounds beneficial for use in cosmetic products such as skin care and personal care products. These products may be in the form of a cream, lotion, bar or stick. The compounds of formula I or II have new and unexpected properties as cosmetic additives not only as an emollient but also as solvents and liquid carriers for a cosmetically active material in the cosmetic preparation.

Esters of the first aspect may be made by analogous esterification reactions to those used for the preparation of other fatty alcohol-aromatic acid esters.

20

In accordance with a preferred embodiment of this invention, the ester is suitably free of other fatty alcohol or fatty acid esters; and is suitably in a substantially pure state.

In accordance with a second aspect of the present invention there is provided a composition for application to the person, for example to hair, skin or nails, the composition comprising as one component an ester of the first aspect. Said composition may hereinafter be called a cosmetic composition or a topical composition or a skin benefit composition.

5

Further components of the composition may comprise a carrier or diluent or solvent; and/or a cosmetically effective ingredient. Such further components may be as hereinafter described.

5 Preferably the composition of the second aspect constitutes at least 40 %wt, preferably at least 50 %wt, more preferably at least 70 %wt, most preferably at least 90 %wt, of the total weight of $C_{12}-C_{15}$ fatty alcohol-aromatic acid ester content in the composition. Most preferably the composition is substantially free of $C_{12}-C_{15}$ fatty alcohol-aromatic acid esters apart from compound(s) of the first aspect.

In certain embodiments the composition of the second aspect constitutes at least 40 %wt, preferably at least 50 %wt, more preferably at least 70 %wt, most preferably at least 90 %wt, of the total weight of all esters of fatty alcohols and acids in the composition. Most preferably the composition is substantially free of all esters of fatty alcohols and acids apart from the compound(s) of the first aspect.

20

25

30

15

The esters of the first aspect have valuable properties. The representative compound of formula II is substantially nongreasy, shows lack of oiliness and greasiness, has very low cloud point and pour point, has a bland odor, low toxicity and is stable. The representative compound of formula II has good tactile properties, spreadibility, solubility in/with sunscreen agents, low tackiness (stickiness), low greasiness on the skin, good suspension properties (TiO_2) and is effective in wetting and dispersing pigments. These properties make it useful as vehicle or carrier emollient or solubilizer for toiletry and cosmetic formulations such as sunscreen creams, hair creams, hand creams, cold creams, manual and electric pre-, during- and post-shave

6

compositions, fingernail polish, topical pharmaceutical ointments, lipsticks, skin lotion and creams, as well as other formulations. A particular use for the esters of the first aspect of this invention is as emollients for antiperspirant, deodorant, sun-screening and personal cleansing compositions. The ester of formula I or II, when added to cosmetic compositions, incorporates in the cosmetic composition one or more, or all, of the following features:

Ease of emulsification;

High refractive index;

5

25

30

Emolliency with good after feel;

Lack of greasiness/pleasant skin feel;

Lack of oiliness while imparting good lubrication;

Low cloud point and pour point;

15 High spreading coefficient;

Alcohol solubility;

Low toxicity;

Hydrolytic stability; and

Solvent for many skin and hair additives including

sunscreens.

An ester of the first aspect has properties in addition to those mentioned hereinbefore when used as an emollient in a sunscreen agent. In this regard, it has been found that when ester of the first aspect is incorporated as an emollient in a sunscreen agent, it increases the sun protection factor ("SPF") of the sunscreen agent in these sunscreen compositions. In this manner, one achieves in a sunscreen composition containing the ester of the first aspect, a sun protecting effect not only due to the sunscreen agent but also due to the ester of the first aspect. Therefore, sunscreen agents of a lower sun protecting factor can be utilized in sunscreen compositions containing an

5

10

15

20

7

ester of the first aspect and achieve the sunscreen protecting factors of higher protecting sunscreen agents.

For best results, as ester of the first aspect should be added to a composition when it is substantially pure and substantially free of other esters of aromatic acids with fatty alcohols. In this manner, it is believed that best results are achieved. However, this should not preclude the use of other fatty acid esters or fatty acids in these compositions, suitably within the percentage limits mentioned above, since the use of the novel ester may still provide enhanced results to cosmetic compositions in which it is incorporated.

An ester of the first aspect may be incorporated into cosmetic or skin treating compositions as an emollient in order to impart to these compositions the aforementioned beneficial properties of this invention. The ester of the first aspect can be used as an ingredient for any topical cosmetic compositions including skin, nail, lip, hair topical compositions not only as an emollient but as a diluent, solvent and liquid carrier. As a solvent, an ester of the first aspect is an effective solubilizer for the cosmetically active agents used in these cosmetic compositions.

25 In accordance with this invention, an ester of the first aspect of this invention is suitably incorporated in a cosmetic composition in an emollient effective amount. In this manner, the ester is provided in an amount at least sufficient to provide the emollient properties to the cosmetic composition.

30 Emollients are dermatologically acceptable compositions that tend to lubricate the skin, increase the softness and suppleness of the skin, prevent or relieve dryness of the skin and/or

8

protect the skin. These emollients are typically water emissible, oily or waxy material and in order to provide the improved results of this invention, an ester of the first aspect may be supplied as an additive to these cosmetic compositions in an amount which is at least sufficient to provide or improve the emollient properties to the cosmetic composition. In accordance with this invention an ester of the first aspect can suitably be added to the cosmetic composition in any amount which is at least sufficient impart emolliency to to the composition. The amount of this mixture used in these cosmetic compositions depends on the type and quantity of ingredients used and in the amount and type of functional additives that are utilized. Generally the amount of the ester of this invention that is incorporated into these cosmetic compositions ranges from about 0.1% to about 30% by weight, for example about 0.3% to about 20% by weight, based upon the total weight of the cosmetic composition, with amounts from about 5% to about 15% by weight based upon the weight of the composition being especially preferred.

20

25

30

5

10

15

In a third aspect of the present invention there is provided a method of preparing a cosmetic composition, wherein an ester of the first aspect of this invention mixed with other ingredients so as to produce a cosmetic composition of the second aspect of this invention.

An ester of the first aspect can be utilized to produce the beneficial properties set forth above in any conventional topical cosmetic composition such sunscreen creams, hair creams, hand ointments, lipsticks, skin lotions and creams as well as other formulations. The term cosmetic compositions include both cosmetic, skin care as well as lip, hair and nail compositions

9

which are topically applied to the humans to achieve a beneficial action on the surface to which it is applied.

An ester of the first aspect is advantageous in that it may be one or more of non-oily, tasteless, inert, essentially nontoxic and non sensitizing, and stable. The ester of the first aspect may provide one or more of emollient, solubilizer, moisturizer, plasticizer, sunscreen vehicle/solvent, de-oiler/degreaser, and emulsifier/co-emulsifier properties. An ester of the first aspect may possess unusual physico-chemical properties, in particular, excellent spreading coefficient which can make it beneficial and unique component of sophisticated delivery system such as in hand, face, and body creams, lotions, soaps and sticks.

15

20

25

30

10

5

Further an ester of the first aspect may be a solvent and/or vehicle for solid organic ultraviolet (UV) absorbers. It may have a function as a plasticizer for polymers contained in skin care composition, and acts as auxiliary suspending agents capable of assisting in the suspension of ingredients in skincare composition and also may function as a dye leveling agent and dye carrier. Thus, an ester of the first aspect when used in a skin care composition may serve not only as an emollient, but also as a carrier; and it may also exhibit these other functions.

In accordance with this invention, the cosmetic composition whose properties may be enhanced by the addition of the ester of the first aspect of the invention can be any conventional cosmetically active material which provides a therapeutic or beneficial cosmetic action to the human body particularly the skin, lips hair or nails. These cosmetic compositions can be in

WO 2009/083735

5

10

10

PCT/GB2008/051227

the form of a cream, lotion, ointment, spray, soap-bar, stick etc. which contain a cosmetically active material. In accordance with this invention the term cosmetically active materials may include anti-aging ingredients, anti-wrinkling agents, minerals, preservatives, antioxidants, moisturizers, vitamins, sunscreen agents, and anti-acne agents, deodorants, antiperspirants etc. Among the preferred cosmetically active material are vitamins such as Vitamin A, B₁, B₂, B₃, B₅, B₆, B₁₂, biotin, Vitamin C, Vitamin D, Vitamin E, folic acid and Vitamin K. Other preferred cosmetically active ingredients which can be utilized in the cosmetic composition of this invention anti wrinkling agents, anti-acne agents, moisturizers such as Vitamin E, mineral oils, diisopropyl adipate.

If the cosmetic composition of the second aspect is in the form 15 of a liquid, it may contain a liquid aqueous carrier medium for the cosmetic composition. The liquid aqueous carrier medium can be water or it can be an oil in water or oil in water liquid emulsion. In accordance with this invention, any cosmetically acceptable carrier which is compatible with the water can be 20 combined with water to form the aqueous carrier medium of the second component system. The aqueous carrier medium can contain one or more oil components. The oil component may be any pharmaceutically or cosmetically acceptable oily material which is substantially insoluble in water. These materials can be 25 found for example in the CTFA International Dictionary of Cosmetic Ingredients as well as the U.S. Pharmacopoeia or other equivalent sources. Suitable oil components include, but are not limited to, natural oils, such as coconut oil; hydrocarbons, such as mineral oil and hydrogenated polyisobutene; sterol 30 derivatives, such as lanolin; animal waxes, such as beeswax, plant waxes, such as carnauba; mineral waxes, such as ozokerite;

11

petroleum waxes, such as paraffin wax; synthetic waxes, such as polyethylene; and mixtures thereof. If the cosmetic composition is in the form of a solid, such as a deodorant stick, bar or soap, it generally contains a solid carrier medium in the cosmetic composition. Any conventional solid carrier medium used to formulate such solid cosmetic compositions can be used in accordance with this invention.

The cosmetic composition of the second aspect may contain in addition stable ingredients which include various antioxidants, stabilizers, moisturizers, preservatives and emulsifiers such as those mentioned hereinbefore. Any conventional antioxidant, moisturizer, stabilizer, preservative, or emulsifier which is stable in the carrier medium can be present.

15

20

25

30

10

5

To the cosmetic compositions of the second aspect, there may be added known conventional cosmetic additives, adjuvants and vehicle substrates. Emulsifiers such as glycerol stearate or methyl glucose sesquistearate may also be present Also present may be organic solvents, such as lower aliphatic alcohols from 1 to 6 carbon atoms, such as ethanol isopropanol or propanol, or glycols such as glycerin or 1,2-propylene glycol. The following can also be included in the final cosmetic product: perfume oils; opacifiers such as ethylene glycol distearate; wetting agents or emulsifiers; anti-bacterial and fungicidal ingredients; thickeners (such as bentonite); pH substances; moisture retaining agents; fragrances or perfumes; perfume oils; colorants (such as natural or synthetic direct dyes but also tinting agents such as fluorescein sodium salt); sunscreens or UV filters; preservatives; antioxidants (such as tocopherols); pyrogemic silicic acid; complexing agents; and also physiologically tolerable inorganic or organic acids, such

12

as phosphoric acid, acetic acid, formic acid, glyoxylic acid, lactic acid, tartaric acid or citric acid; bases; salts (such as sodium chloride); buffers (such as sodium citrate or sodium phosphate); consistency-lending agents; and natural, modified, partly or entirely synthetic polymers (such as chitosan, FMOC chitosan and PVP). Naturally, one skilled in the art will be familiar with which of the various individual adjuvants and vehicle substances to be added in order to obtain a desired formulation of the composition of this invention. However, in accordance with a preferred aspect of this invention, these composition preferably do not contain fatty alcohol esters, other than those of the first aspect of this invention; or if present such further esters are present within limits set out hereinabove.

15

10

5

In accordance with a fourth aspect of the present invention there is provided a method of treating the skin or hair of a person using an ester of an optionally substituted aromatic acid and a branched C_{13} primary alcohol.

20

25

In accordance with a fifth aspect of the present invention there is provided the use of an ester of an optionally substituted aromatic acid and a branched C_{13} primary alcohol for any purpose or to achieve any benefit stated herein; and particularly but not exclusively for providing one or more of improved sunscreening, improved moisturizing and improved emolliency.

Preferred features of the first and second aspects are also preferred features of the third, fourth or fifth aspects.

30

This invention is further illustrated by the following Examples.

13

In the Examples Additive A is a C_{13} benzoate ester prepared by esterifying 1 mole of isotridecane-1-ol (Marlipal O13) with 1 mole of benzoic acid (i.e. unsubstituted) under standard esterification conditions. The resulting product had an acid value below 0.1 mg KOH/g and had been filtered through a filter press with Whatman Paper No. 4. Additive A was an odourless liquid with a freezing point of -25°C, refractive index of 1.4850 and specific gravity of 0.903 at 25°C.

5

10 In the Examples, the chemical names of the trade or generic names set forth in the Examples are illustrated in Table I as follows:

Table I Identification Of Trade Or Generic Listed Preparation Ingredients

Trade or Generic Material	Identification	Source
Marlipal 013 alcohol	Isotridecane-1-ol	Sasol North America Inc.
Aminol HCA	Cocoamide dimethicone PEG/PPG-20/30	Innospec Performance Chemicals
Finsolv SLB-101	Hydrophilic alkoxylated benzoate ester	Innospec Performance Chemicals
Finsolv SLB-201	Dimethicone PEG-8 benzoate	Innospec Performance Chemicals
Finsolv TN	C12 - C15 alkyl benzoate	Innospec Performance Chemicals
Finester EH 25	C12 - C15 alkyl octanoate	Innospec Performance Chemicals
Finester LP	Di C12 - C15 alkyl maleate	Innospec Performance Chemicals
Finsolv PL-62	Poloxamer 182 dibenzoate	Innospec Performance Chemicals
Finester DOM-R	Dioctyl maleate	Innospec Performance Chemicals
Finsolv EMG.20	Methyl gluceth - 20 benzoate	Innospec Performance Chemicals
Finsolv PL-355	Poloxamer 105 benzoate	Innospec Performance Chemicals
Finsolv BCO-115	Castor oil benzoate	Innospec Performance Chemicals
Finsolv BCR-111	Cetyl ricinoleate	Innospec Performance Chemicals
Finsolv BOHS-111	Ethylhexyl hydroxy stearate benzoate	Innospec Performance Chemicals

Crothix	PEG-150 pentaerythritol tetrastearate	Innospec Performance Chemicals
Tauranol I 78 C	Sodium cocyl isethionate	Innospec Performance Chemicals
Tauranol WS (conc)	Sodium methyl cocyl taurate	Innospec Performance Chemicals
Surfine - AZI-A	Nonoxynol-10 carboxylic acid	Innospec Performance Chemicals
Natrlfine 137-T	Behenyl benzoate, titanium dioxide	Innospec Performance Chemicals
Solulan 16	Laureth-16, Ceteth-16, Oleth 16 and Steareth-16	Amerchol Edison
Drakeol 9	Light mineral oil	Panorco
Hystrene 9718	Stearic acid ethylene diamine	Witco Corporation
Hampine Na 4	Tetraacetic acid, sodium salt	Hampshire Chemical Corp.
Polyglycol E400	Polyethylene glycol 400	D.V.C. Limited Inc.
Sodium stearate C7	Sodium stearate	Witco Corporation
Dow Corning Fluid 344	Cyclomethicone	Dow Corning
Dow Corning Fluid 200	Dimethicone	Dow Corning
Carbomer	Carbopol ETD 2001 resin	B.F. Goodrich
Brij 78	Steareth-20	ICI
Triclosan	Igason DP 300	Ciba Geigy
Dow Corning Fluid 345	Cyclomethicone	Dow Corning
Adol 62	Stearyl alcohol	Witco Corporation
Castor Wax MP 70	Hydrogenated castor oil	Cas Chemical

16

Reach AZP 908	Aluminum zirconium tetrachloro-glycine complex	Reheis Inc.
Silica	Cabosil M-5	Cabot Corp.
Germaben II	Diazolidinyl urea	ISP (NJ, USA)
Escalol 567	Benzophenone-3	ISP
Escalol 587	Octylmethoxycinnamate	ISP
Witconol 2314	Isopropyl myristate	Witco Corporation
Witconol 2316	Isopropyl palmitate	Witco Corporation
Finsolv SB	Isostearyl benzoate	Innospec Performance Chemicals
Finsolv PG22	Dipropylene glycol dibenzoate	Innospec Performance Chemicals
Finsolv BOD	Octyldodecyl benzoate	Innospec Performance Chemicals

EXAMPLE 1

Solubility and compatibility of Additive A

5

10

The solubility characteristics of Additive A are tabulated below. It is soluble at normal handling and use temperatures in most commonly used solvents, emollients and vehicles employed in cosmetic product formulations.

	Water	_
	Ethanol	+
	Isopropanol	+
5	Mineral Oil	_
	Glycerin	_
	Propylene glycol	_
	Dimethicone copolyol (Silwet 7604, 7230)	+
	Cyclomethicone (Dow Corning Fluid 244)	_
10	Dimethicone (Dow Corning fluid 200)	_
	Isopropyl myristate	+
	Isopropyl palmitate	+
	Finsolv SLB101	+
	Finsolv SLN 201	+
15	Finsolv PL 62	+
	Finsolv PL 355	+
	Finsolv BCO 115	+
	Finsolv BCR 111	+
	Finsolv BOHS 111	+
20	Finsolv TN	+
	Finsolv TPP	+
	Finsolv EMG 20	+
	Finsolv BOD	+
25	Finsolv SB	+
25	Finsolv PG22	+
	Finester EH 25	+
	Finester DOM-R	+

30 Key: "+" indicates soluble at ambient temperatures
"-" indicates insoluble at ambient temperatures

18

EXAMPLE 2

Sunscreen Solubilities in Esters (25°C)

5

10

15

25

The two most commonly used solid organic crystalline sunscreens are 2 hydroxy-4-methoxybenzophenone (called Benzophenone-3) and Parsol 1789 (butyl-methoxy dibenzoyl methane). These two sunscreens are difficult to dissolve and keep in solution for use in sunscreen formulations for optimal SPF (Sun - Protection Factors). Higher solvency for a sunscreen ingredient is described as it allows higher concentrations of the sunscreen active ingredient in a formulation. This advantageously raises the SPF ratings for the formulations. The liquid organic sunscreens that are commonly used as octylsalicylate (OS) and octyl-methoxycinnamate (OMC). Esters of this invention exhibit superiority over commonly used and marketed cosmetic emollients/materials.

Sunscreen	Solubility in	Solubility in	Solubility in
	Additive A	Finsolv TN	Finester LP
	(%)	(%)	(%)
Benzophenone-3	25	15	10
Parsol 1789	23	13	6

20 The high solvency exhibited by the Additive A for the solid crystalline organic sunscreens is an advantageous effect in formulating sunscreen products for the skin care markets. Thus, besides being cosmetic emollients, it is excellent solvent for the above-mentioned sunscreens.

A further aspect of this ester, besides being solubilizers for the sunscreens, renders antiwashoff effects. This effect is

19

very attractive in formulating long lasting sunscreen products allowing the sunscreen to remain on the skin for a longer duration.

5 EXAMPLE 3

Sunscreen Cream

A sunscreen cream was prepared from the following ingredients with the amounts set forth in the table being percent by weight:

Ingredient/Trade	A	В	С	D	E	F
name						
I.						
Water	62	62	62	62	62	62
Polyglycol E-400	5	5	5	5	5	5
II.						
Additive A	7			_	_	-
Finsolv TN	-	7	_	_	_	_
Finester EH-25	-	_	7	_	_	_
Finester LP	-	_	_	7	_	_
Witconol 2314	-	_	_	_	7	_
Finester DOM-R	-	_	_	_	_	7
Finsolv EMG-20	6	6	6	6	6	6
Parsol MCX	8	8	8	8	8	8
Escalol 567	3	3	3	3	3	3
Escalol 587	5	5	5	5	5	5
Crothix	1	1	1	1	1	1
Cetal	1	1	1	1	1	1
Cerasynt SD	1	1	1	1	1	1
III.						
Germaben	1	1	1	1	1	1

WO 2009/083735

20

PCT/GB2008/051227

The sunscreen cream was prepared from the ingredients set forth above by the following procedure:

- 1. Charge the ingredients of Part I starting with water.
- 2. Bring the temperature to 70°C to 75°C.
- 3. Mix well until uniform.

5

15

20

- 4. Heat ingredients of Part II to 75°C.
- 5. Add ingredients of Part II to Part I with mixing.
- 6. Cool to 35°C with gentle mixing.
- 7. Add ingredient of Part III.
 - 8. Mix well and cool to 30°C.

Each product was evaluated against Additive A. The amount of sample used was 0.5 cc product administered by syringe. Each product was evaluated for the following attributes and rated on a scale of 1 to 5, whereas 1 being the best. Each product was timed from moment of application to the end feel and judged on its absorption time. The above products were applied onto the forearm and the opposite hand rubbing into the skin using 4 fingers, evaluating each sample. The forearm was evaluated with warm water and wipe dry before evaluating another set of samples. This procedure and scale is used in the rest of the examples in this application

25 Formulations A to F so prepared were tested for skin feel, emolliency, slip and spreadibility on a scale of 1 to 5 with 1 representing the best and 5 representing poor. Results are as follows:

21

Ingredients/Trade Name	A	В	С	D	E	F
Skin feel	1	3	4	4	5	5
Emolliency	1	3	3	4	5	5
Slip	1	3	4	4	5	5
Spreadability	1	3	3	4	5	5

EXAMPLE 4

Sunscreen Stick

A sunscreen stick was prepared from the following ingredients with the amounts set forth in the table being percent by weight:

Ingredients/Trade Name	A	В	С	D	E	F
Witconol APM	44	44	44	44	44	44
Additive A	25	_	_	_		_
Finsolv TN	-	25	_	_	_	_
Finester EH-25	_	_	25	_	_	_
Finester LP	_	_	_	25	_	_
Witconol 2314	_	_	_	_	25	_
Finester DOM-R	_	_	_	_	_	25
Parsol MCX	7.5	7.5	7.5	7.5	7.5	7.5
Escalol 587	5.5	5.5	5.5	5.5	5.5	5.5
Sodium stearate C7	8	8	8	8	8	8
Aminol HCA	7	7	7	7	7	7
Water	3	3	3	3	3	3

22

The sunscreen stick was prepared from the ingredients set forth above by the following procedure:

- 1. Charge the ingredients in descending order.
- 2. Bring the temperature to 80°C.
 - 3. Mix well until uniform.
 - 4. Cool to 60°C.
 - 5. Pour into appropriate molds at 60°C.
- 10 Formulations A to F so prepared were tested for slip, spreadibility, skin feel, emolliency, stickiness and water rinse off resistance on a scale of 1 to 5 with 1 representing the best and 5 representing poor. Results are as follows:

Ingredients/Trade Name	A	В	С	D	E	F
Slip	1	2	3	4	5	5
Spreadability	1	3	3	4	5	4
Skin feel	1	3	3	4	5	5
Emolliency	1	3	4	4	5	5
Stickiness	1	3	4	4	5	4
Water rinse-off resistance	1	3	4	4	5	5

23

EXAMPLE 5

Clear Sunscreen Oil

A clear sunscreen oil was prepared from the following 5 ingredients with the amounts set forth in the table being percent by weight:

Ingredients/Trade Name	A	В	С	D	E	F
I.						
Dow Corning fluid 344	60	60	60	60	60	60
Dow Corning fluid 200	10	10	10	10	10	10
II.						
Additive A	10	_	_	_	_	_
Finsolv TN	-	10	_	_	_	_
Finester EH-25	_	_	10	_	_	_
Finester LP	_	_	_	10	_	_
Witconol 2314	_	_	_	_	10	_
Finester DOM-R	_	_	_	_	_	10
Parsol MCX	8	8	8	8	8	8
Escalol 567	4	4	4	4	4	4
Escalol 587	8	8	8	8	8	8

The clear sunscreen oil was prepared from the ingredients set 10 forth above by the following procedure:

- 1. Mix the ingredients of Part I & II separately, until uniform.
- 2. When uniform added II to I and stir at 25°C.

24

All formulations are clear liquid at 25°C. Formulation A to F so prepared were tested for slip, water rinse off resistance, stickiness, feel and emolliency. On a scale of 1 to 5 with 1 representing the best and 5 representing poor. Results are as follows:

Ingredients/Trade Name	A	В	С	D	E	F
Slip	1	2	3	4	5	5
Water rinse-off resistance	1	3	3	4	5	4
Stickiness	1	3	3	4	5	4
Feel	1	2	3	4	5	5
Emolliency	1	2	3	4	5	4

EXAMPLE 6 Moisturizing Hand and Body Lotion

A moisturizing hand and body lotion was prepared from the following ingredients with the amounts set forth in the table being percent by weight:

Ingredients/Trade Name	A	В	С	D	E	F
I.						
Water	85.95	85.95	85.95	85.95	85.95	85.95
Carbomer	0.15	0.15	0.15	0.15	0.15	0.15
Methylparaben	0.1	0.1	0.1	0.1	0.1	0.1
Propylparaben	0.1	0.1	0.1	0.1	0.1	0.1
Sorbitol 70	2	2	2	2	2	2
Hampine Na	0.2	0.2	0.2	0.2	0.2	0.2
Triethanolamine	0.9	0.9	0.9	0.9	0.9	0.9
II.						
Additive A	5	_	_	_	_	_
Finsolv TN	_	5	_	_	_	_
Finester EH-25	-	_	5	_	_	_
Finester LP	_	_	_	5	_	_
Witconol 2314	_	-	_	_	5	_
Finester DOM-R	_	_	_	_	_	5
Dracol 9	1.6	1.6	1.6	1.6	1.6	1.6
Cetal	0.7	0.7	0.7	0.7	0.7	0.7
Hysterene 9718	1.5	1.5	1.5	1.5	1.5	1.5
Cerysynt SD	0.8	0.8	0.8	0.8	0.8	0.8
Promulgen G	1	1	1	1	1	1

26

The moisturizing hand and body lotion was prepared from the ingredients set forth above by the following procedure:

- 1. Charge water and disperse Carbomer in it.
- 2. Charge balance of Part I ingredients in order each to dissolve.
 - 3. After addition of triethanolamine, heat to 65°C.
 - 4. Mix Part I ingredients together and heat to 60°C.
 - 5. Add Part II ingredients to Part I ingredients with good mixing to form emulsion.
 - 6. Continue mixing while cooling to 25°C. All formulations are opaque flowable lotion with pH 6.5.

Formulations A to F so prepared were tested for skin feel, slip, stickiness, long lasting moisturizing effect and emolliency using a scale of 1 to 5 with 1 representing the best and 5 representing poor. Results are as follows:

Ingredients/Trade Name	A	В	С	D	E	F
Skin	1	2	3	4	5	5
Slip	1	2	3	4	5	5
Stickiness	1	2	3	4	5	4
Moisturizing effect	1	2	3	3	5	5
Emolliency	1	2	3	4	5	4

5

27

EXAMPLE 7 Elegant Skin Crème

A elegant skin crème was prepared from the following ingredients with the amounts set forth in the table being percent by weight:

A	В	С	D	E	F
75.4	75.4	75.4	75.4	75.4	75.4
1.2	1.2	1.2	1.2	1.2	1.2
0.2	0.2	0.2	0.2	0.2	0.2
1.8	1.8	1.8	1.8	1.8	1.8
5	5	5	5	5	5
1	1	1	1	1	1
0.8	0.8	0.8	0.8	0.8	0.8
2.6	2.6	2.6	2.6	2.6	2.6
3	3	3	3	3	3
9	_	_	_	_	_
-	9	_	_	_	_
-	_	9	_	_	_
_	_	_	9	_	_
_	_	_	_	9	_
-	_	_	_	_	9
	75.4 1.2 0.2 1.8 5 1 0.8 2.6 3	75.4 75.4 1.2 1.2 0.2 0.2 1.8 1.8 5 5 1 1 0.8 0.8 2.6 2.6 3 3 9 -	75.4 75.4 75.4 1.2 1.2 1.2 0.2 0.2 0.2 1.8 1.8 1.8 5 5 5 1 1 1 0.8 0.8 0.8 2.6 2.6 2.6 3 3 3 9 - 9 - - 9 - - 9	75.4 75.4 75.4 75.4 1.2 1.2 1.2 1.2 0.2 0.2 0.2 0.2 1.8 1.8 1.8 1.8 5 5 5 5 1 1 1 1 0.8 0.8 0.8 0.8 2.6 2.6 2.6 2.6 3 3 3 3 9 9 9 9	75.4 75.4 75.4 75.4 75.4 75.4 1.2 1.2 1.2 0.2 0.2 0.2 0.2 0.2 1.8 1.8 1.8 1.8 1.8 5 5 5 5 5 5 1 1 1 1 1 1 0.8 0.8 0.8 0.8 0.8 0.8 2.6 2.6 2.6 2.6 2.6 3 3 3 3 3 3 3 9

The skin crème was prepared from the ingredients set forth above by the following procedure:

- 1. Charge the ingredients of Part I starting with water.
- 2. Bring the temperature to 70° C to 75° C.

28

- 3. Mix well until uniform.
- 4. Heat ingredients of Part II to 75°C.
- 5. Add ingredients of Part II to Part I with mixing.

6. Cool to 25°C with gentle mixing.

5

All formulations are soft in appearance and are of pH 6.6. Formulations A to F so prepared were tested for skin feel, slip, stickiness, emolliency, on a scale of 1 to 5 with 1 representing the best and 5 representing poor. The results are as follows:

10

Ingredients/Trade Name	A	В	С	D	E	F
Skin feel	1	2	3	4	5	5
Slip	1	2	3	4	5	5
Stickiness	1	2	3	4	5	5
Emolliency	1	2	3	4	5	5

EXAMPLE 8

Deodorant Stick

15

A deodorant stick was prepared from the following ingredients with the amounts set forth in the table being percent by weight:

Ingredients / Trade Name	A	В	С	D	E	F
Propylene glycol	65	65	65	65	65	65
Water	15	15	15	15	15	15
Sodium stearate C7	8	8	8	8	8	8
Brij 78	8	8	8	8	8	8
Additive A	3.8	_	_	-	_	_
Finsolv TN	_	3.8	-	_	_	_
Finester EH25	_	_	3.8	_	_	_
Finester LP	-	_	_	3.8	_	_
Witconol 2314	_	_	_	_	3.8	_
Finester DOM-R	_	_	-	_	_	3.8
Triclosan	0.2	0.2	0.2	0.2	0.2	0.2

The deodorant stick was prepared from the ingredients set forth above by the following procedure:

- 5 1. Change the ingredients in descending sequence starting with propylene glycol.
 - 2. Bring the temperature to 80°C allowing all to dissolve.
 - 3. Mix well until uniform.
 - 4. Cool to 60°C and cast into stick molds.

10

Formulations A to F so prepared were tested for emolliency, slip, soft dry and afterfeel using a scale of 1 to 5 with 1 representing the best and 5 representing poor. Results as follows:

Ingredients/Trade Name	A	В	С	D	E	F
Emolliency	1	2	3	3	5	4
Slip	1	2	2	3	5	4
Soft dry after-feel	1	2	2	3	5	4

30

EXAMPLE 9 Non-Whitening Antiperspirant Stick

A non-whitening antiperspirant stick was prepared from the 5 following ingredients with the amounts set forth in the table being percent by weight:

Ingredients / Trade Name	A	В	С	D	E	F
I.						
Dow Corning 345 Fluid	39	39	39	39	39	39
Adol 62	18	18	18	18	18	18
Castorwax MP-70	5	5	5	5	5	5
Additive A	5	_	_	-	-	_
Finsolv TN	-	5	-	_	-	-
Finester EH 25	_	_	5	_	_	-
Finester LP	_	_	_	5	_	-
Witconal 2314	_	_	_	-	5	_
Finester DOM-R	_	_	_	_	_	5
Finsolv 116	10	10	10	10	10	10
II.						
Reach AZP - 908	20	20	20	20	20	20
Talc	2	2	2	2	2	2
Silica	1	1	1	1	1	1

- 10 The non-whitening antiperspirant stick was prepared from the ingredients set forth above by the following procedure:
 - 1. Charge the ingredients of Part I starting with Dow Corning Fluid 345.
 - 2. Bring the temperature to 75°C.

31

- 3. Mix well until uniform.
- 4. Add Part II powders, mix until completely dispersed.

 Maintain 75°C.
- 5. Cool to 55°C and cast in to stick molds.

5

Formulation A to F so prepared were tested for emolliency, stickiness, talc like feel, and stick structure. On a scale of 1 to 5 with 1 representing the best and 5 representing poor. The results are as follows:

10

Ingredients/Trade Name	A	В	С	D	E	F
Emolliency	1	2	3	3	5	4
Stickiness	1	2	2	3	5	5
Talc-like feel	1	2	2	3	5	4
Stick structure	1	2	3	3	5	5

15 General comment applicable throughout

In this specification, including in the examples, percentage values are expressed in terms of weight by total composition weight (wt/wt) unless otherwise stated.

32

Claims

1. An ester of an optionally substituted aromatic acid and a branched C_{13} primary alcohol.

5

- 2. An ester as claimed in claim 1 wherein the optionally substituted aromatic acid is optionally substituted benzoic acid.
- 10 3. An ester as claimed in claim 1 or 2 wherein the aromatic acid is unsubstituted.
 - 4. An ester as claimed in any preceding claim wherein the branched C_{13} primary alcohol residue is branched from one position only, on the backbone of the primary alcohol.
 - 5. An ester as claimed in any preceding claim wherein the branched C_{13} primary alcohol residue contains from 1 to 6 carbon atoms, preferably a methyl group, in one or more side chains.

20

15

6. An ester as claimed in any preceding claim wherein the branched C_{13} primary alcohol residue is branched from the penultimate carbon atom in the backbone, with reference to the optionally substituted aromatic moiety.

25

7. An ester as claimed in any preceding claim having the formula

8. An ester as claimed in any preceding claim provided in at least 90% by weight pure form, preferably at least 95%, preferably at least 98%, preferably substantially pure.

9. A composition for application to the person, the composition comprising as one component an ester as claimed in any of claims 1 to 8.

10

5

10. A composition as claimed in claim 9 comprising a carrier or diluent or solvent; and/or a cosmetically effective ingredient, for example a sunscreen agent, and a deodorant agent or an antiperspirant agent.

15

20

- 11. A composition as claimed in claim 9 or 10 wherein said ester constitutes at least 40 %wt, preferably at least 50 %wt, more preferably at least 70 %wt, most preferably at least 90 %wt, and preferably substantially all, of the total weight of $C_{12}-C_{15}$ fatty alcohol-aromatic acid ester content in the composition.
- 12. A composition as claimed in claim 9 or 10 wherein said ester constitutes at least 40 %wt, preferably at least 50 %wt, more preferably at least 70 %wt, most preferably at least 90 %wt, and preferably substantially all, of the total weight of all esters of fatty alcohols and acids in the composition.

34

- 13. A composition as claimed in any of claims 9 to 12 wherein said ester is present in the amount of from about 0.1% to about 30% by weight, based upon the total weight of the composition.
- 5 14. A composition as claimed in any of claims 9 to 13 wherein said ester functions in the composition as an emollient and is the only emollient present in the composition.
- 15. A composition as claimed in any of claims 9 to 14 wherein the composition is a sunscreen composition and contains a sunscreen agent whose effectiveness is enhanced by said ester.
 - 16. A method of preparing a composition as claimed in any of claims 9 to 15 wherein an ester as claimed in any of claims 1 to 8 is mixed with other ingredients so as to produce said composition.

- 17. A method of treating the skin or hair of a person using an ester of an optionally substituted aromatic acid and a branched c_{13} primary alcohol.
- 18. Use of an ester of an optionally substituted aromatic acid and a branched C_{13} primary alcohol, for providing one or more of improved sunscreening, improved moisturizing and improved emolliency.

INTERNATIONAL SEARCH REPORT

International application No PCT/GB2008/051227

Relevant to claim No.

A. CLASSIFICATION OF SUBJECT MATTER INV. C07C69/78 A61K8/00

C. DOCUMENTS CONSIDERED TO BE RELEVANT

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Category*

 $\begin{array}{ll} \text{Minimum documentation searched (classification system followed by classification symbols)} \\ \text{C07C} & \text{A61K} \end{array}$

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, CHEM ABS Data, BEILSTEIN Data, WPI Data

Citation of document, with indication, where appropriate, of the relevant passages

X	US 2007/060768 A1 (GRASS MICHAEL AL) 15 March 2007 (2007-03-15) example 4	[DE] ET	1-8
X	US 5 922 900 A (WIELAND STEFAN [D 13 July 1999 (1999-07-13) column 3, line 58	E] ET AL)	1,2,4 - 6, 8
Y	US 2005/014961 A1 (WALELE ISMAIL AL) 20 January 2005 (2005-01-20) claims 1-27; tables I-X	I [US] ET	1–18
Y	US 5 959 130 A (WALELE ISMAIL [US 28 September 1999 (1999-09-28) claims 1-5; tables I-V	[] ET AL)	1–18
* Special of Course consider the Course which citation other the Course	ent defining the general state of the art which is not lered to be of particular relevance document but published on or after the international date ent which may throw doubts on priority claim(s) or is cited to establish the publication date of another nor other special reason (as specified) ent referring to an oral disclosure, use, exhibition or means ent published prior to the international filing date but	T* later document published after the inte or priority date and not in conflict with cited to understand the principle or the invention TX* document of particular relevance; the cannot be considered novel or cannot involve an inventive step when the do TY* document of particular relevance; the cannot be considered to involve an inventive step when the do TY* document of particular relevance; the cannot be considered to involve an indeximent is combined with one or ments, such combined with one or ments, such combination being obvious in the art. Take the patent family annex.	the application but early underlying the claimed invention be considered to current is taken alone claimed invention wentive step when the ore other such docurrent to a person skilled
2	0 May 2009	02/06/2009	
Name and r	nailing address of the ISA/ European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31–70) 340–2040, Fax: (+31–70) 340–3016	Authorized officer Butkowskyj-Walkiw	, T-

INTERNATIONAL SEARCH REPORT

International application No
PCT/GB2008/051227

C(Continua	tion). DOCUMENTS CONSIDERED TO BE RELEVANT	
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Υ	WO 02/051788 A (GIVAUDAN SA [CH]; MCGEE THOMAS [US]; PURZYCKI KENNETH LEO [US]; VEDANT) 4 July 2002 (2002-07-04) claims 1-19; examples 1-8	1-18
Y	US 4 275 222 A (SCALA JR THOMAS L) 23 June 1981 (1981-06-23) cited in the application the whole document	1-18
	,	

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No PCT/GB2008/051227

	t document search report		Publication date		Patent family member(s)		Publication date
US 20	07060768	A1	15-03-2007	DE EP WO US	10347863 1682480 2005037764 2008245996	A1 A1	04-05-2005 26-07-2006 28-04-2005 09-10-2008
US 59	22900	A	13-07-1999	CA DE EP JP ZA	2214491 19635769 0827947 10095747 9707915	A1 A1 A	04-03-1998 05-03-1998 11-03-1998 14-04-1998 02-03-1998
US 20	05014961	A1	20-01-2005	NONE		<u></u>	
US 59	59130	Α	28-09-1999	NONE			
WO 02	051788	A	04-07-2002	BR CA CN CN EP MX US	0116345 2428903 1481351 1721001 1345883 PA03005658 2003008787	A1 A A A1 A	25-02-2004 04-07-2002 10-03-2004 18-01-2006 24-09-2003 03-12-2004 09-01-2003
US 42		<u>-</u>	23-06-1981	NONE			