

Recognized as Safe as a flavor ingredient – GRAS 3. (2456)

Other Actions

Indicative Non-Exhaustive List	of fragrance ingredients
Joint Expert Committee on Food Additives	No safety concern at current levels of intake. (1997)

FFIDS Volume I

Hazard Statements

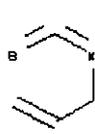
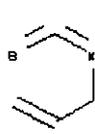
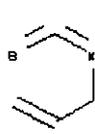
1-Jan-01	S33	Take precautionary measures against static discharges.	
1-Jan-01	S29	Do not empty into drains.	
1-Jan-01	S24	Avoid contact with skin.	
1-Jan-01	S23	Do not breathe gas/fumes/vapour/spray (appropriate wording to be specified by the manufacturer).	
1-Jan-01	S16	Keep away from sources of ignition No smoking.	
1-Jan-01	R11	Highly flammable.	 Highly Flammable
1-Apr-89		Liquid and vapor may be irritating to skin and eyes.	
1-Apr-89		Breathing high concentrations of vapor may cause anesthetic effects.	

Human Health Data

Environmental Data

Other References to Ethyl propionate

RIFM – FEMA Database

Allyl isothiocyanate																
RIFM – FEMA Database																
Comprehensive Computer Generated Synopsis																
Skip To – <ul style="list-style-type: none"> • Physical Data • Flavor • Consumption • Food Uses • Food Products • Status • Hazards • Human Health Data • Environmental Data • Other References 	<table border="1" style="width: 100%;"> <tr> <td colspan="2">Synonyms</td> <td rowspan="7" style="text-align: center; vertical-align: middle;">  </td> </tr> <tr> <td colspan="2">AITC</td> </tr> <tr> <td colspan="2">Allyl isosulfocyanate</td> </tr> <tr> <td>Allyl isothiocyanate</td> <td>Principal</td> </tr> <tr> <td colspan="2">Allyl thiocarbonimide</td> </tr> <tr> <td>1-Propenal, 3-isothiocyanato-</td> <td>CAS</td> </tr> <tr> <td colspan="2">2-Propenyl isothiocyanate</td> </tr> </table>	Synonyms			AITC		Allyl isosulfocyanate		Allyl isothiocyanate	Principal	Allyl thiocarbonimide		1-Propenal, 3-isothiocyanato-	CAS	2-Propenyl isothiocyanate	
	Synonyms															
	AITC															
	Allyl isosulfocyanate															
	Allyl isothiocyanate	Principal														
	Allyl thiocarbonimide															
	1-Propenal, 3-isothiocyanato-	CAS														
	2-Propenyl isothiocyanate															
	CAS Number FEMA EINECS Registration 57-06-7 2034 200-309-2 EINECS DSL TSCA															
	Formula C_4H_5NS Structure $CH_2=CH-CH_2-N=C=S$ Molecular Weight 99.16															
SMILES Notation $N(=C=S)CC=C$																
Generic Class (TSCA) Sulfur Containing Compounds																
Description Colorless or pale yellow, very refractive liquid with very pungent, irritating odor and acrid taste, lachrymatory, tends to darken on aging																
Physical Data																
<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 30%;">Boiling Point</td> <td style="width: 30%;">150-C</td> <td style="width: 40%;">FMA</td> </tr> <tr> <td>Flash Point</td> <td>111-F;CC</td> <td>FMA</td> </tr> <tr> <td>Log K_{ow} (calculated)</td> <td>2.15</td> <td>Syracuse Research Corp.</td> </tr> <tr> <td>Specific Gravity</td> <td>1.018</td> <td>FMA</td> </tr> </table>		Boiling Point	150-C	FMA	Flash Point	111-F;CC	FMA	Log K_{ow} (calculated)	2.15	Syracuse Research Corp.	Specific Gravity	1.018	FMA			
Boiling Point	150-C	FMA														
Flash Point	111-F;CC	FMA														
Log K_{ow} (calculated)	2.15	Syracuse Research Corp.														
Specific Gravity	1.018	FMA														
<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 20%;">Preparation</td> <td>By distillation of sodium thiocyanate and allyl chloride (Fenaroli,1971)</td> </tr> <tr> <td>Natural Occurrence</td> <td>Allyl isothiocyanate is reported to occur in nature.</td> </tr> </table>		Preparation	By distillation of sodium thiocyanate and allyl chloride (Fenaroli,1971)	Natural Occurrence	Allyl isothiocyanate is reported to occur in nature.											
Preparation	By distillation of sodium thiocyanate and allyl chloride (Fenaroli,1971)															
Natural Occurrence	Allyl isothiocyanate is reported to occur in nature.															
Flavor Consumption (in kg)																

1995	USA	1009
1995	EUROPE	10524
1987	USA	17300
1982	USA	15300
1976	USA	6850
1975	USA	8070
1970	USA	21400

Uses (in ppm)

Product	Average Usual	Average Maximum	Mean Daily Consumption (gms)	Updated
Baked Goods	25.0	100.0	137.2	28-Jul-88
Condiment Relish	718.0	5000.0	8.8	28-Jul-88
Fats Oils	49.99	50.0	17.5	21-Jul-88
Fish Products	0.05	0.07	12.4	28-Jul-88
Frozen Dairy	0.0	0.0	25.6	28-Jul-88
Gelatin Pudding	1.0	2.0	20.4	21-Jul-88
Gravies	2.0	10.0	8.3	16-Jun-89
Meat Products	35.22	61.16	78.4	21-Jul-88
Non-alcoholic Beverage	1.0	2.0	104.0	21-Jul-88
Processed Vegetables	30.0	50.0	85.0	28-Jul-88
Seasonings Flavors	6.5	30.0	0.01	28-Jul-88
Snack Foods	48.0	100.0	1.1	28-Jul-88
Soft Candy	1.6	3.5	5.8	28-Jul-88

PADI 16.13

Food Products Containing Allyl isothiocyanate (in ppm)

Product	Code	Lower Limit	Upper Limit
Unknown	106-A	0.06	
Cabbage (raw)	18-I	0.04	2.9
Cabbage (cooked)	18-II	0.2	0.3

Status

Allyl isothiocyanate was included by the Council of Europe in the list of substances granted Not in 4th edition - reason unknown (COE No. 2110) .

Allyl isothiocyanate was approved by the FDA as GRAS Affirmation proposed 8/26/77 184.1527 (21 CFR 172.515) .

Allyl isothiocyanate was listed by the IARC as follows: There is limited evidence for the carcinogenicity of allyl isothiocyanate to experimental animals. There is inadequate evidence in humans for the carcinogenicity of allyl isothiocyanate. Allyl isothiocyanate is not classifiable as to its carcinogenicity to humans (Group 3). (IARC 1999, vol 73, pg 37) .

Allyl isothiocyanate has an IFRA Standard: Prohibited. Should not be used as a fragrance ingredient. Based on the absence of reports on its use as a fragrance ingredient and inadequate evaluation of possible physiological effects resulting from its use in fragrances. (8904) .

Flavor and Extract Manufacturers' Association states: Generally Recognized as Safe as a flavor ingredient - GRAS 3. (2034)

FFIDS Volume I

Hazard Statements

1-Jan-01	S45	In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).	
1-Jan-01	S36/37	Wear suitable protective clothing and gloves.	
1-Jan-01	S28	After contact with skin, wash immediately with plenty of...(to be specified by the manufacturer).	
1-Jan-01	S26	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.	
1-Jan-01	R36/37/38	Irritating to eyes, respiratory system and skin.	 Irritant
1-Jan-01	R23/24/25	Toxic by inhalation, in contact with skin and if swallowed.	 Toxic
1-Jan-01	R(10)	Flammable (Unless indicated otherwise by the manufacturer)	
5-Feb-91		Inhalation of vapors causes irritation of the pulmonary tract.	
1-Apr-89		Toxic. May cause serious health effects if swallowed.	
1-Apr-89		Very toxic. Skin contact may be fatal.	
1-Apr-89		Irritating to the skin and eyes.	

National Toxicology Program

1		Last Update 16-Feb-99	Report Published
	Carcinogenicity gavage rat		Report published. Positive evidence of carcinogenicity in male rats & equivocal evidence in female rats.
2		Last Update 16-Feb-99	Report Published
	Carcinogenicity gavage mouse		Report published - No evidence of carcinogenicity in male & female mice.
<p><u>Human Health Data</u> <u>Environmental Data</u></p> <p><u>Other References to Allyl isothiocyanate</u></p> <p><u>RIFM - FEMA Database</u></p>			

Ethyl acetoacetate

RIFM – FEMA Database

Comprehensive Computer Generated Synopsis

Skip To –

- [Physical Data](#)
- [Flavor](#)
- [Consumption](#)
- [Food Uses](#)
- [Status](#)
- [Hazards](#)
- [Human Health Data](#)
- [Environmental Data](#)
- [Other](#)
- [References](#)

Synonyms

Acetoacetic ester

Butanoic acid, 3-oxo-, ethyl ester

Ethyl acetoacetate

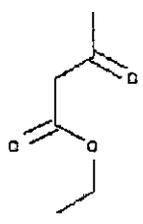
Ethyl acetylacetate

Ethyl β-ketobutyrate

Ethyl 3-oxobutanoate

CAS

Principal EINECS RIFM



CAS Number 141-97-9 RIFM ID 390 FEMA 2415 EINECS 205-516-1 Registration EINECS DSL TSCA

RIFM Monograph: 390 (Published 1974: FCT,v12,p713 (Binder, p343))

Formula C₆H₁₀O₃ Structure CH₃-CO-CH₂-OCO-CH₂-CH₃
 Molecular Weight 130.14
 SMILES Notation O=C(OCC)CC(=O)C
 Generic Class (TSCA) Aliphatic Esters
 Description Food Chemicals Codex (1972)

Physical Data

Boiling Point	181-C	FMA
Flash Point	183-F;CC	FMA
Log K _{ow} (calculated)	-0.2	Syracuse Research Corp.
Specific Gravity	1.025	FMA
Vapor Pressure (calculated)	0.5 mm Hg 20C	FMA

Preparation	From ethyl acetate by the action of sodium, sodium ethoxide, sodamide or calcium (Merck Index,1968)
Natural Occurrence	Ethyl acetoacetate is reported to occur in nature.
Use Levels	In public use since the 1950s.

Flavor Consumption (in kg)

1995	USA	32821
1995	EUROPE	9734
1987	USA	20500
1982	USA	17100
1976	USA	27600
1975	USA	10300
1970	USA	6170

Uses (in ppm)

Product	Average Usual	Average Maximum	Mean Daily Consumption (gms)	Updated
Alcoholic Beverage	0.0066	0.0066	32.5	29-Jul-88
Baked Goods	465.0	1000.0	137.2	16-Jun-89
Breakfast Cereals	2.0	100.0	20.0	29-Jul-88
Chewing Gum	10.0	41.0	0.2	16-Jun-89
Confection Frosting	400.0	800.0	0.3	29-Jul-88
Frozen Dairy	0.2	0.7	25.6	29-Jul-88
Fruit Ices	10.0	100.0	0.7	29-Jul-88
Fruit Juice	0.1	1.0	118.3	29-Jul-88
Gelatin Pudding	51.0	520.0	20.4	16-Jun-89
Hard Candy	25.79	53.22	0.6	21-Jul-88
Jam Jelly	280.0	980.0	5.7	29-Jul-88
Meat Products	42.6	70.5	78.4	21-Jul-88
Milk Products	5.0	100.0	39.5	29-Jul-88
Non-alcoholic Beverage	154.0	2100.0	104.0	29-Jul-88
Seasonings Flavors	10.0	30.0	0.01	29-Jul-88
Snack Foods	18.0	18.0	1.1	29-Jul-88
Soft Candy	140.0	1300.0	5.8	16-Jun-89
Sweet Sauce	1.0	14.0	6.8	29-Jul-88

PADI 87.02

Status

Ethyl acetoacetate was included by the Council of Europe in the list of substances granted B – information required – hydrolysis studies on 2 substances of CE nos: 227, 240–244 (FEMA 3551, 2415, 2176, 2177, 2510 or 2136) (COE No. 240) .

Ethyl acetoacetate was approved by the FDA as a flavor (21 CFR 172.515) .

Flavor and Extract Manufacturers' Association states: Generally Recognized as Safe as a flavor ingredient – GRAS 3. (2415)

Other Actions

Indicative Non-Exhaustive List of fragrance ingredients

FFIDS Volume II

Hazard Statements

20-Nov-01	NL	Based on available data, an IFRA/IOFI/EFFA classification and labeling was not considered necessary. Labeling Manual, March 2001
1-Apr-89		Vapor is irritating to throat and lungs.
1-Apr-89		Liquid may be irritating to skin. Eye irritant.

Human Health Data
Environmental Data

Other References to Ethyl acetoacetate

RIFM – FEMA Database

資料 21

Evaluation of certain food additives and contaminants
(Forty-ninth, Fifty-first, Fifty-third, and Fifty-fifth report
of the Joint FAO/WHO Expert Committee on Food Additives). WHO
Technical Report Series.

Table 1
Summary of the results of safety evaluations of 38 saturated aliphatic acyclic linear primary alcohols, aldehydes and acids^a

Substance	No.	Step A3 ^b Does intake exceed the threshold for human intake?	Step A4 Endogenous or metabolized to endogenous substances?	Comments	Conclusion based on levels of current intake
Formic acid ^c	0079	No Europe: 800 USA: 160	NR	Formic acid is produced endogenously in humans and is a normal component of intermediate metabolism	No safety concern
Acetaldehyde	0080	Yes Europe: 11000 USA: 9700	Yes	Acetaldehyde is oxidized to acetic acid which is metabolized via the citric acid cycle; acetaldehyde can also be reduced to ethanol	
Acetic acid ^c	0081	Yes Europe: ND USA: 360000	Yes	Acetic acid is metabolized to carbon dioxide; it acetylates amines and can be incorporated into proteins	
Propyl alcohol	0082	Yes Europe: 420 USA: 2700	Yes	Propyl alcohol is oxidized to propionaldehyde which is oxidized to propionic acid; propionic acid is metabolized via the citric acid cycle	
Propionaldehyde	0083	No Europe: 33 USA: 140	NR	Propionaldehyde is oxidized to propionic acid which is metabolized via the citric acid cycle	

Propionic acid ^d	0084	Yes Europe: 1100 USA: 5200	Yes	Propionic acid is metabolized via the citric acid cycle	No safety concern
Butyl alcohol	0085	Yes Europe: 1900 USA: 8100	Yes	Butyl alcohol is oxidized to butyraldehyde which is oxidized to butyric acid; butyric acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Butyraldehyde	0086	No Europe: 26 USA: 17	NR	Butyraldehyde is oxidized to butyric acid which is metabolized via the fatty acid and tricarboxylic acid pathways	
Butyric acid	0087	Yes Europe: 10000 USA: 5900	Yes	Butyric acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Amyl alcohol	0088	No Europe: 97 USA: 44	NR	Amyl alcohol is oxidized to valeraldehyde which is rapidly oxidized to valeric acid; valeric acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Valeraldehyde	0089	Yes Europe: 3000 USA: 8.8	Yes	Valeraldehyde is rapidly oxidized to valeric acid which is metabolized via the fatty acid and tricarboxylic acid pathways	
Valeric acid	0090	No Europe: 140 USA: 850	NR	Valeric acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Hexyl alcohol	0091	Yes Europe: 1900 USA: 800	Yes	Hexyl alcohol is oxidized to hexanal which is rapidly oxidized to hexanoic acid; hexanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Hexanal	0092	No Europe: 780 USA: 260	NR	Hexanal is rapidly oxidized to hexanoic acid which is metabolized via the fatty acid and tricarboxylic acid pathways	
Hexanoic acid	0093	Yes Europe: 3500 USA: 1300	Yes	Hexanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	

Table 1 (continued)

Substance	No.	Step A3 ^b Does intake exceed the threshold for human intake?	Step A4 Endogenous or metabolized to endogenous substances?	Comments	Conclusion based on current levels of intake
Heptyl alcohol	0094	No Europe: 12 USA: 7	NR	Heptyl alcohol is oxidized to heptanal which is rapidly oxidized to heptanoic acid; heptanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	No safety concern
Heptanal	0095	No Europe: 200 USA: 3.2	NR	Heptanal is rapidly oxidized to heptanoic acid which is metabolized via the fatty acid and tricarboxylic acid pathways	
Heptanoic acid	0096	No Europe: 170 USA: 5.3	NR	Heptanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
1-Octanol	0097	No Europe: 230 USA: 32	NR	1-Octanol is oxidized to octanal which is rapidly oxidized to octanoic acid; octanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Octanal ^c	0098	No Europe: 170 USA: 90	NR	Octanal is rapidly oxidized to octanoic acid which is metabolized via the fatty acid and tricarboxylic acid pathways	
Octanoic acid	0099	Yes Europe: 3800 USA: 650	Yes	Octanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Nonyl alcohol	0100	No Europe: 8.1 USA: 2.1	NR	Nonyl alcohol is oxidized to nonanal which is rapidly oxidized to nonanoic acid; nonanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Nonanal ^c	0101	No Europe: 130 USA: 17	NR	Nonanal is rapidly oxidized to nonanoic acid which is metabolized via the fatty acid and tricarboxylic acid pathways	

Nonanoic acid	0102	No Europe: 64 USA: 63	NR	Nonanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	No safety concern
1-Decanol	0103	No Europe: 290 USA: 7	NR	1-Decanol is oxidized to decanal which is rapidly oxidized to decanoic acid; decanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Decanal	0104	No Europe: 288 USA: 61	NR	Decanal is rapidly oxidized to decanoic acid which is metabolized via the fatty acid and tricarboxylic acid pathways	
Decanoic acid	0105	No Europe: 1400 USA: 980	NR	Decanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways; at high concentrations, it undergoes ω -oxidation	
Undecyl alcohol	0106	No Europe: 0.9 USA: 11	NR	Undecyl alcohol is oxidized to undecanal which is rapidly oxidized to undecanoic acid; undecanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Undecanal	0107	No Europe: 480 USA: 1.5	NR	Undecanal is rapidly oxidized to undecanoic acid which is metabolized via the fatty acid and tricarboxylic acid pathways	
Undecanoic acid	0108	No Europe: 4.6 USA: 8.8	NR	Undecanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Lauryl alcohol	0109	No Europe: 170 USA: 80	NR	Lauryl alcohol is oxidized to lauric aldehyde which is rapidly oxidized to lauric acid; lauric acid is metabolized via the fatty acid and tricarboxylic acid pathways	

Table 1 (continued)

Substance	No.	Step A3 ^b Does intake exceed the threshold for human intake?	Step A4 Endogenous or metabolized to endogenous substances?	Comments	Conclusion based on current levels of intake
Lauric aldehyde	0110	No Europe: 52 USA: 21	NR	Lauric aldehyde is rapidly oxidized to lauric acid which is metabolized via the fatty acid and tricarboxylic acid pathways	No safety concern
Lauric acid	0111	No Europe: 590 USA: 1200	NR	Lauric acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Myristaldehyde	0112	No Europe: 9.4 USA: 25	NR	Myristaldehyde is rapidly oxidized to myristic acid which is metabolized via the fatty acid and tricarboxylic acid pathways	
Myristic acid	0113	No Europe: 160 USA: 72	NR	Myristic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
1-Hexadecanol	0114	No Europe: 3.6 USA: 0.2	NR	1-Hexadecanol is oxidized to hexadecanal which is rapidly oxidized to hexadecanoic acid; hexadecanoic acid is metabolized via the fatty acid and tricarboxylic acid pathways	
Palmitic acid	0115	No Europe: 89 USA: 234	NR	β -oxidation of palmitic acid yields 2-carbon units which enter the tricarboxylic acid cycle	
Stearic acid	0116	Yes Europe: 58 USA: 1900	Yes	β -oxidation of stearic acid yields 2-carbon units which enter the tricarboxylic acid cycle	

NR: Not required for evaluation because consumption of the substance was determined to be of no safety concern at step A3 of the procedure. ND: no intake data reported.

^a Step 1: All of the substances in this group are in structural class 1, the human intake threshold of which is 1800 μ g per day.

^b Step 2: All of the substances in this group are metabolized to innocuous products.

^c All intake values are expressed in μ g per day.

^d The ADI for this substance was maintained.

Table 3
Summary of the results of safety evaluations of 35 aliphatic lactones

Substance	No.	Step 2 Metabolized to innocuous products?	Step A3/B3 ^a Does intake exceed the threshold for human intake?	Step A4 Is the substance or are its metabolites endogenous?	Step B4/A5 Adequate NOEL for substance or related substance?	Conclusion based on current levels of intake
Structural class I						
4-Hydroxybutyric acid lactone (γ -butyrolactone)	0219	Yes	No Europe: 130 USA: 100	NA	NA	No safety concern
γ -Valerolactone	0220	Yes	No Europe: 140 USA: 57	NA	NA	
γ -Hexalactone	0223	Yes	No Europe: 190 USA: 19	NA	NA	
δ -Hexalactone	0224	Yes	No Europe: 380 USA: 2.5	NA	NA	
γ -Heptalactone	0225	Yes	No Europe: 190 USA: 41	NA	NA	

Table 3 (continued)

Substance	No.	Step 2 Metabolized to innocuous products?	Step A3/B3 ^a Does intake exceed the threshold for human intake?	Step A4 Is the substance or are its metabolites endogenous?	Step B4/A5 Adequate NOEL for substance or related substance?	Conclusion based on current levels of intake
γ -Octalactone	0226	Yes	No Europe: 490 USA: 90	NA	NA	No safety concern
δ -Octalactone	0228	Yes	No Europe: 270 USA: 17	NA	NA	
γ -Nonalactone ^b	0229	Yes	No Europe: 1200 USA: 470	NA	NA	
Hydroxynonanoic acid δ -lactone	0230	Yes	No Europe: 150 USA: 11	NA	NA	
γ -Decalactone	0231	Yes	Yes Europe: 1800 USA: 370	No	Yes	
δ -Decalactone	0232	Yes	Yes Europe: 8400 USA: 1900	No	Yes	
ϵ -Decalactone	0241	Yes	No Europe: 0.01 USA: 0	NA	NA	
γ -Undecalactone ^b	0233	Yes	No Europe: 1400 USA: 550	NA	NA	

5-Hydroxyundecanoic acid δ -lactone	0234	Yes	No Europe: 350 USA: 180	NA	NA
γ -Dodecalactone	0235	Yes	No Europe: 220 USA: 110	NA	NA
δ -Dodecalactone	0236	Yes	Yes Europe: 6800 USA: 1140	No	Yes
ϵ -Dodecalactone	0242	Yes	No Europe: 0.01 USA: 0.17	NA	NA
δ -Tetradecalactone	0238	Yes	No Europe: 120 USA: 2.5	NA	NA
ω -Pentadecalactone	0239	Yes	No Europe: 84 USA: 51	NA	NA
4-Hydroxy-3-pentenoic acid lactone	0221	Yes	No Europe: NR USA: 4.8	NA	NA
5-Hydroxy-7-decenoic acid δ -lactone	0247	Yes	No Europe: 0.26 USA: 0.10	NA	NA

Table 3 (continued)

Substance	No.	Step 2 Metabolized to innocuous products?	Step A3/B3 ^a Does intake exceed the threshold for human intake?	Step A4 Is the substance or are its metabolites endogenous?	Step B4/A5 Adequate NOEL for substance or related substance?	Conclusion based on current levels of intake
5-Hydroxy-8-undecenoic acid δ -lactone	0248	Yes	No Europe: 0.01 USA: 8.6	NA	NA	No safety concern
1,4-Dodec-6-enolactone	0249	Yes	No Europe: 0.01 USA: 8.6	NA	NA	
ω -6-Hexadecenolactone	0240	Yes	No Europe: 6 USA: 0.10	NA	NA	
4,4-Dibutyl- γ -butyrolactone	0227	Yes	No Europe: 0.14 USA: 0.10	NA	NA	
3-Heptyldihydro-5-methyl-2(3H)- furanone	0244	Yes	No Europe: 0.04 USA: 0.1	NA	NA	
4-Hydroxy-3-methyloctanoic acid γ -lactone	0437	Yes	No Europe: 0 USA: 8.6	NA	NA	
6-Hydroxy-3,7-dimethyloctanoic acid lactone	0237	Yes	No Europe: 0.1 USA: 0	NA	NA	
γ -Methyldecalactone	0250	Yes	No Europe: 0 USA: 43	NA	NA	

Structural class III							
5-Hydroxy-2-decenoic acid δ -lactone	0246	No	No Europe: 12 USA: 0.10	NA	Insufficient information	Not evaluated ^c	
5-Hydroxy-2,4-decadienoic acid δ -lactone	0245	No	No Europe: 0.33 USA: 0.10	NA	Insufficient information		
Mixture of 5-hydroxy-2-decenoic acid δ -lactone, 5-hydroxy-2-dodecenoic acid δ -lactone and 5-hydroxy-2-tetradecenoic acid δ -lactone	0276	No	— Europe: 0 USA: 2	NA	Insufficient information		
5-Hydroxy-2-dodecenoic acid δ -lactone	0438	No	— Europe: 0 USA: 8.6	NA	Insufficient information	No safety concern	
5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	0222	No	No Europe: 13 USA: 6.1	NA	Yes		
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one	0243	No	No Europe: 2.1 USA: 0.1	NA	Yes		

NA: not applicable.

^a The thresholds for human intake for classes I and III are 1800 μg per day and 90 μg per day, respectively. All intake values are expressed in μg per day.

^b The ADI for this substance was maintained.

^c Evaluation deferred, pending consideration of other α,β -unsaturated compounds.

Table 4

Summary of the results of safety evaluations of 32 esters of aliphatic acyclic primary alcohols with branched-chain aliphatic acyclic acids^a

Substance	No.	Step A3 ^b Does intake exceed the threshold for human intake?	Step A4 Endogenous or metabolized to endogenous substances?	Conclusion based on current levels of intake
Methyl isobutyrate	0185	No Europe: 23 USA: 270	NR	No safety concern
Ethyl isobutyrate	0186	No Europe: 750 USA: 470	NR	
Propyl isobutyrate	0187	No Europe: 15 USA: 0.08	NR	
Butyl isobutyrate	0188	No Europe: 2.7 USA: 1.9	NR	
Hexyl isobutyrate	0189	No Europe: 3.00 USA: 0.57	NR	
Heptyl isobutyrate	0190	No Europe: 0.00 USA: 3.0	NR	
<i>trans</i> -3-Heptenyl 2- methylpropanoate	0191	No Europe: 0.01 USA: 2.3	NR	
Octyl isobutyrate	0192	No Europe: 11 USA: 5.0	NR	
Dodecyl isobutyrate	0193	No Europe: 50 USA: 0.76	NR	
Isobutyl isobutyrate	0194	No Europe: 65 USA: 2.3	NR	
Methyl isovalerate	0195	No Europe: 7.8 USA: 110	NR	
Ethyl isovalerate	0196	No Europe: 760 USA: 540	NR	
Propyl isovalerate	0197	No Europe: 2.00 USA: 0.10	NR	
Butyl isovalerate	0198	No Europe: 94 USA: 500	NR	
Hexyl 3-methyl- butanoate	0199	No Europe: 2.3 USA: 3.1	NR	
Octyl isovalerate	0200	No Europe: 7.3 USA: 0.57	NR	
Nonyl isovalerate	0201	No Europe: 0.01 USA: 0.08	NR	