



Name: R_INQUIRY / SUBSTANCE : Fatty acids, C14-18 and C16-18-unsatd. / (9Z)-octadec-9-enoic acid; hexadecanoic acid; o... Thu, 17 May 2018 09:36:10 +0000

Legal entity owner: EcoMundo for twin rivers / Issy-les-Moulineaux / France

Printing date: 2018-05-17T09:36:33.245Z

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DOSSIER:

UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.377Z

Remarks:

Dossier header

Dossier submission type

Name

REACH Inquiry

Version

reach 3.0

Dossier subject

Dossier subject

[Fatty acids, C14-18 and C16-18-unsatd. / \(9Z\)-octadec-9-enoic acid; hexadecanoic acid; octadecanoic acid / 67701-06-8](#)

Submitting legal entity

[EcoMundo for twin rivers / Issy-les-Moulineaux / France](#)

Dossier creation date/time

Thu May 17 09:36:10 GMT 2018

Used in category

false

LEGAL_ENTITY: EcoMundo for twin rivers

UUID: ECHA-3df66680-b937-4ffb-8b8c-d2cbd4c23c47

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.389Z

Remarks:

General information

Legal entity name

EcoMundo for twin rivers

Legal entity type

company

Contact information

Contact address

Address 1

215 Rue Jean Jacques Rousseau

Postal code

92130

Town

Issy-les-Moulineaux

Country

France

Phone

0033183642054

E-mail

or@ecomundo.eu

Fatty acids, C14-18 and C16-18-unsatd.

General information

Identification

SUBSTANCE: Fatty acids, C14-18 and C16-18-unsatd.

UUID: af11c3ed-52bf-4c93-9285-34dff1af8655

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.436Z

Remarks:

Substance name

Fatty acids, C14-18 and C16-18-unsatd.

Legal entity

[EcoMundo for twin rivers / Issy-les-Moulineaux / France](#)

Contact persons

Person

[Garçon, Pierre; EcoMundo](#)

Last name

Garçon

First name

Pierre

Organisation

EcoMundo

Phone

00 33 (0)1 83 64 20 53

Email

or@ecomundo.eu

Address 1

215, rue Jean-Jacques Rousseau

Postal code

92130

Town

Issy-les-Moulineaux

Country

France

Identification of substance

Reference substance

[Fatty acids, C14-18 and C16-18-unsatd. / \(9Z\)-octadec-9-enoic acid; hexadecanoic acid; octadecanoic acid / 67701-06-8 / 266-930-6](#)

EC number

266-930-6

EC name

EC Inventory

CAS number

67701-06-8

CAS name

IUPAC name

(9Z)-octadec-9-enoic acid; hexadecanoic acid; octadecanoic acid

Type of substance

Type of substance

UVCB

Origin

organic

Role in the supply chain

Manufacturer

false

Importer

false

Only representative

true

Downstream user

false

Composition

FLEXIBLE_RECORD: Composition.001

UUID: 96212934-ff6b-4e58-ba26-4d2a4e07f3ff

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.455Z

Remarks:

General Information

Name

Fatty acids, C14-18 and C16-18-unsatd.

Type of composition

legal entity composition of the substance

State / form

solid: bulk

Description

DESCRIBE THE PROCESS BEHIND THE PARTICULAR COMPOSITION OF THE UVCB SUBSTANCE

- Identity of starting materials/source (and ratio):

Coconut oil or tallow/water

- Reaction steps/mechanisms:

1. Hydrolysis

2. Distillation

3. Fractionation

4. Hydrogenation

- Relevant operating parameters (e.g. temperature and pressure):

350F-450F

- Solvents/reagents used:

None (water)

- Details on any extraction/isolation steps as appropriate: None

- Details on any clean-up/purification steps as appropriate: Distillation

- Physical-chemical parameters (e.g. boiling point):

pH: 3 - 4

Boiling point/Boiling range: >464F (240C) @ 15 mm Hg

Flash Point & Method: ~356F (>180C) ASTM D 92

Degree of purity

100

% (w/w)

Constituents

Reference substance

[\(E\)-octadec-11-enoic acid / octadec-11-enoic acid / 693-72-1 / 211-758-9](#)

EC number

211-758-9

EC name

EC Inventory

CAS number 693-72-1	CAS name octadec-11-enoic acid
IUPAC name octadec-11-enoic acid	
Typical concentration ca. 29.83	% (w/w)
Concentration range >= 5	<= 70 % (w/w)
Reference substance myristic acid / Tetradecanoic acid / 544-63-8 / 208-875-2	
EC number 208-875-2	EC name EC Inventory
CAS number 544-63-8	CAS name Tetradecanoic acid
IUPAC name Tetradecanoic acid	
Typical concentration ca. 5.16	% (w/w)
Concentration range >= 0	<= 10 % (w/w)
Reference substance (Z)-hexadec-9-enoic acid / hexadec-9-enoic acid / 373-49-9 / 206-765-9	
EC number 206-765-9	EC name EC Inventory
CAS number 373-49-9	CAS name hexadec-9-enoic acid
IUPAC name hexadec-9-enoic acid	
Typical concentration ca. 2.61	% (w/w)
Concentration range >= 0	<= 5 % (w/w)

Reference substance[palmitic acid / Hexadecanoic acid / 57-10-3 / 200-312-9](#)**EC number**

200-312-9

EC name

EC Inventory

CAS number

57-10-3

CAS name

Hexadecanoic acid

IUPAC name

Hexadecanoic acid

Typical concentration

ca. 22.36 % (w/w)

Concentration range

>= 5 <= 65 % (w/w)

Reference substance[heptadecanoic acid / heptadecanoic acid / 506-12-7 / 208-027-1](#)**EC number**

208-027-1

EC name

EC Inventory

CAS number

506-12-7

CAS name

heptadecanoic acid

IUPAC name

heptadecanoic acid

Typical concentration

ca. 2.14 % (w/w)

Concentration range

>= 0 <= 5 % (w/w)

Reference substance[stearic acid / Octadecanoic acid / 57-11-4 / 200-313-4](#)**EC number**

200-313-4

EC name

EC Inventory

CAS number

57-11-4

CAS name

Octadecanoic acid

IUPAC name

Octadecanoic acid

Typical concentration

ca. 23.04 % (w/w)

Concentration range

>= 5 <= 55 % (w/w)

Reference substance

[9-octadecenoic acid / octadec-9-enoic acid / 2027-47-6 / 217-977-6](#)

EC number

217-977-6

EC name

EC Inventory

CAS number

2027-47-6

CAS name

octadec-9-enoic acid

IUPAC name

octadec-9-enoic acid

Typical concentration

ca. 10.13 % (w/w)

Concentration range

>= 5 <= 70 % (w/w)

Analytical information

FLEXIBLE_RECORD: Analytical information.001

UUID: 4d14529e-0c1f-4bd6-a42b-6ad47b723a8d

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.436Z

Remarks:

Analytical information

Methods and results of analysis

Analytical determination

Purpose of analysis

identification and quantification

Analysis type

chromatography – GC

IR

MS

NMR

UV/Vis

Type of information provided

methods and results

Attached methods/results

4_EC 266-930-6_V2.pdf / 3.577 MB (application/pdf)

Optical activity

no

Information requirements

Inquiry

FLEXIBLE_RECORD: Inquiry.001

UUID: 964d3f13-99a4-434d-82dc-49662d311028

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.452Z

Remarks:

Type of inquiry

Specify the type of inquiry

Type 3: Inquiry for phase-in substance that has not been pre-registered

Information requirements

Information requirements requiring new studies to be conducted?

no

References

REFERENCE_SUBSTANCE: Fatty acids, C14-18 and C16-18-unsatd.

UUID: 103892f7-baed-4872-801e-686d30100cd0

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.389Z

Remarks:

General information

Reference substance name

Fatty acids, C14-18 and C16-18-unsatd.

Inventory

Inventory name

Fatty acids, C14-18 and C16-18-unsatd.

Inventory

EC

Inventory number

266-930-6

CAS number

67701-06-8

Molecular formula

Description

This substance is identified by SDA Substance Name: C14-C18 and C16-C18 unsaturated alkyl carboxylic acid and SDA Reporting Number: 04-005-00.

Reference substance information

IUPAC name

(9Z)-octadec-9-enoic acid; hexadecanoic acid; octadecanoic acid

CAS information

CAS number

67701-06-8

Molecular and structural information

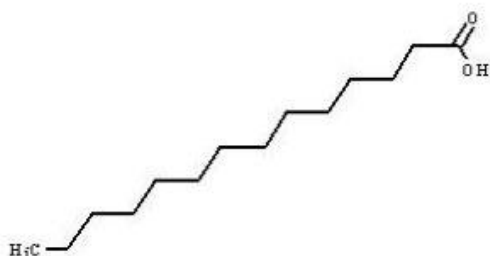
Molecular formula

C52H102O6

SMILES notation

CCCCCCCCCCCCCCCC(O)=O.CCCCCCCCCCCCCCCCCC(O)=O.CCCCCCCC\C=C/CCCC
CCCC(O)=O

Structural formula



MolWt: 228.38 C14 H28 O2
067701-06-8 Fatty acids, C14-18 and C16-18

Remarks

Molecular weight is not applicable as the substance is a UVCB

REFERENCE_SUBSTANCE: (E)-octadec-11-enoic acid

UUID: ECB5-0ab1ed8e-b6ec-46a1-b58e-50ad15066b0c

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.390Z

Remarks:

General information

Reference substance name

(E)-octadec-11-enoic acid

Inventory

Inventory name

(E)-octadec-11-enoic acid

Inventory

EC

Inventory number

211-758-9

CAS number

693-72-1

Molecular formula

C₁₈H₃₄O₂

Description

Reference substance information

IUPAC name

octadec-11-enoic acid

Synonyms

Identity
(e)-octadec-11-enoic_acid
Identity
11-Octadecenoic acid, (E)-

CAS information

CAS number

693-72-1

CAS name

octadec-11-enoic acid

Related substances

Group / category information

DSL Category: Organics

Molecular and structural information

Molecular formula

C₁₈H₃₄O₂

Molecular weight

282.4614

SMILES notation

CCCCC\C=C\CCCCCCCCC(=O)O

InChI

InChI=1/C₁₈H₃₄O₂/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h7-8H,2-6,9-17H₂,1H₃,
(H,19,20)

Structural formula



REFERENCE_SUBSTANCE: (Z)-hexadec-9-enoic acid

UUID: ECB5-ab2cbdde-115e-4321-a63a-58a8d6d0a3e5

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.390Z

Remarks:

General information

Reference substance name

(Z)-hexadec-9-enoic acid

Inventory

Inventory name

(Z)-hexadec-9-enoic acid

Inventory

EC

Inventory number

206-765-9

CAS number

373-49-9

Molecular formula

C₁₆H₃₀O₂

Description

Reference substance information

IUPAC name

hexadec-9-enoic acid

CAS information

CAS number

373-49-9

CAS name

hexadec-9-enoic acid

Molecular and structural information

Molecular formula

C₁₆H₃₀O₂

Molecular weight

254.4082

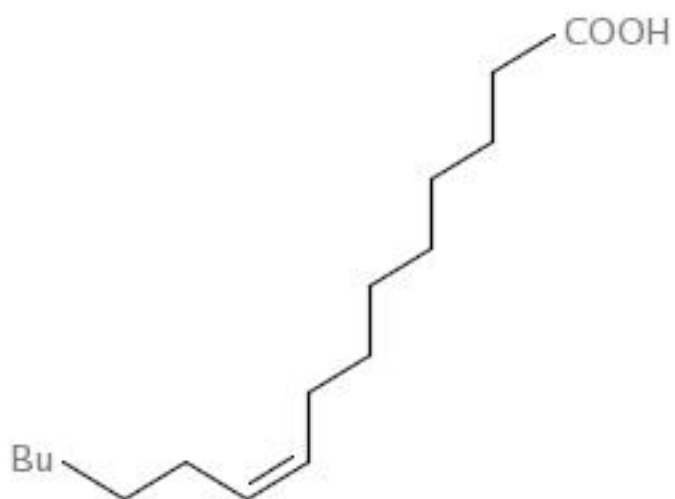
SMILES notation

CCCCC\C=C/CCCCCCC(=O)O

InChI

InChI=1/C16H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h7-8H,2-6,9-15H2,1H3,(H,17,18)

Structural formula



REFERENCE_SUBSTANCE: 9-octadecenoic acid

UUID: ECB5-fb58a8a0-48e6-499d-b764-79dbc8ffd00b

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.391Z

Remarks:

General information

Reference substance name

9-octadecenoic acid

Inventory

Inventory name

9-octadecenoic acid

Inventory

EC

Inventory number

217-977-6

CAS number

2027-47-6

Molecular formula

C₁₈H₃₄O₂

Description

Reference substance information

IUPAC name

octadec-9-enoic acid

Synonyms

Identity
9-Octadecenoic acid
Identity
9-Octadecenoic acid

CAS information

CAS number

2027-47-6

CAS name

octadec-9-enoic acid

Related substances

Group / category information

DSL Category: Organics

Molecular and structural information

Molecular formula

C₁₈H₃₄O₂

Molecular weight

282.4614

SMILES notation

OC(=O)CCCCCCCC=CCCCCCCC

InChI

InChI=1/C₁₈H₃₄O₂/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h9-10H,2-8,11-17H₂,1H₃,(H,19,20)

Structural formula



CONTACT: Garçon, Pierre; EcoMundo

UUID: 969589fe-4a21-3a95-8b1f-55ce3a908bae

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.386Z

Remarks:

General information

Last name

Garçon

First name

Pierre

Organisation

EcoMundo

Phone

00 33 (0)1 83 64 20 53

Email

or@ecomundo.eu

Address 1

215, rue Jean-Jacques Rousseau

Postal code

92130

Town

Issy-les-Moulineaux

Country

France

FR

REFERENCE_SUBSTANCE: heptadecanoic acid

UUID: ECB5-8ecc4c76-75c0-441f-88b0-bad20c8a649b

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.391Z

Remarks:

General information

Reference substance name

heptadecanoic acid

Inventory

Inventory name

heptadecanoic acid

Inventory

EC

Inventory number

208-027-1

CAS number

506-12-7

Molecular formula

C₁₇H₃₄O₂

Description

Reference substance information

IUPAC name

heptadecanoic acid

Synonyms

Identity
Heptadecanoic acid
Identity
Heptadecanoic acid

CAS information

CAS number

506-12-7

CAS name

heptadecanoic acid

Related substances

Group / category information

DSL Category: Organics

Molecular and structural information

Molecular formula

C₁₇H₃₄O₂

Molecular weight

270.4507

SMILES notation

CCCCCCCCCCCCCCCC(=O)O

InChI

InChI=1/C₁₇H₃₄O₂/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19/h2-16H₂,1H₃,(H,18,19)

Structural formula



REFERENCE_SUBSTANCE: myristic acid

UUID: ECB5-da938f82-bb3e-41f5-a652-d5f492b7ba49

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.390Z

Remarks:

General information

Reference substance name

myristic acid

Inventory

Inventory name

myristic acid

Inventory

EC

Inventory number

208-875-2

CAS number

544-63-8

Molecular formula

C₁₄H₂₈O₂

Description

Reference substance information

IUPAC name

Tetradecanoic acid

Synonyms

Identity
Tetradecanoic acid
Identity
Tetradecanoic acid

CAS information

CAS number

544-63-8

CAS name

Tetradecanoic acid

Related substances

Group / category information

DSL Category: Organics

Molecular and structural information

Molecular formula

C₁₄H₂₈O₂

Molecular weight

228.3709

SMILES notation

CCCCCCCCCCCC(=O)O

InChI

InChI=1/C₁₄H₂₈O₂/c1-2-3-4-5-6-7-8-9-10-11-12-13-14(15)16/h2-13H₂,1H₃,(H,15,16)

Structural formula



REFERENCE_SUBSTANCE: palmitic acid

UUID: ECB5-3502c493-86c0-4ed6-a0f9-2cbb8e82cfdc

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.390Z

Remarks:

General information

Reference substance name

palmitic acid

Inventory

Inventory name

palmitic acid

Inventory

EC

Inventory number

200-312-9

CAS number

57-10-3

Molecular formula

C₁₆H₃₂O₂

Description

Reference substance information

IUPAC name

Hexadecanoic acid

Synonyms

Identity Hexadecanoic acid
Identity Hexadecanoic acid
Identity Hexadecanoic acid

CAS information

CAS number

57-10-3

CAS name

Hexadecanoic acid

Related substances

Group / category information

DSL Category: Organics

USEPA Category: Anionic Surfactants

Molecular and structural information

Molecular formula

C₁₆H₃₂O₂

Molecular weight

256.4241

SMILES notation

CCCCCCCCCCCCCCC(=O)O

InChI

InChI=1/C16H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h2-15H2,1H3,(H,17,18)

Structural formula



REFERENCE_SUBSTANCE: stearic acid

UUID: ECB5-ba56bb60-907c-4d3f-8d45-364af5945a64

Dossier UUID: 4d3ea9bd-4526-4c44-b8f3-3b1461718db9

Author: vhajj

Date: 2018-05-17T09:36:10.391Z

Remarks:

General information

Reference substance name

stearic acid

Inventory

Inventory name

stearic acid

Inventory

EC

Inventory number

200-313-4

CAS number

57-11-4

Molecular formula

C₁₈H₃₆O₂

Description

Reference substance information

EU: REACH

IUPAC name

Octadecanoic acid

Synonyms

Identity
Octadecanoic acid
Identity
Octadecanoic acid

CAS information

CAS number

57-11-4

CAS name

Octadecanoic acid

Related substances

Group / category information

DSL Category: Organics

Molecular and structural information

Molecular formula

C₁₈H₃₆O₂

Molecular weight

284.4772

SMILES notation

CCCCCCCCCCCCCCCC(=O)O

InChI

InChI=1/C₁₈H₃₆O₂/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h2-17H₂,1H₃,(H,19,20)

Structural formula

