



---

**Name:** R\_JS\_MBER / SUBSTANCE : C14-C18 FAME Argent Energy - Fatty acids, C14-18 and C16-C18-unsatd., Me esters / UVCB substance, no IUPAC name available chemical name: C14-C18 and 16-C18 unsaturated alkyl carboxyl / 67762-26-9 Thu, 4 Mar 2021, 20:54:12+0000 / FAME Stanlow-OR2

---

**Legal entity owner:**

---

**Printing date:** 2021-03-04T20:54:45.285Z

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# DOSSIER: FAME Stanlow-OR2

---

**UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.213Z

**Remarks:**

---

## Dossier header

---

## Dossier submission type

---

**Name**

REACH Registration member of a joint submission - general case

**Version**

reach 6.0

**Name (given by user)**

FAME Stanlow-OR2

## Dossier subject

---

**Dossier subject**

C14-C18 FAME Argent Energy - Fatty acids, C14-18 and C16-C18-unsatd., Me esters / UVCB substance, no IUPAC name available chemical name: C14-C18 and 16-C18 unsaturated alkyl carboxyl / 67762-26-9

**Public name**

**Submitting legal entity**

**Dossier creation date/time**

Thu, 4 Mar 2021, 20:54:12+0000

**Used in category**

## Type of submission

---

## Tonnage band(s) of the member registrant

---

**Tonnage band**

over 1000 tonnes/year

## Specific submissions

---

**The submission is an update**

true

**Last submission number**

KC774112-54

## Reason for updating

---

---

**Spontaneous update**  
true

**Justification**

<p><b>Justification</b> update following a legal entity change</p>
--

**Dossier specific information**

---

**Phase-in status**  
phase-in

---

# C14-C18 FAME Argent Energy - Fatty acids, C14-18 and C16-C18-unsatd., Me esters

## General information

### Identification

#### Identification

**SUBSTANCE:** C14-C18 FAME Argent Energy - Fatty acids, C14-18 and C16-C18-unsatd., Me esters

---

**UUID:** 03ac9cec-fef7-499a-b953-f202a39e8fa3

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.353Z

**Remarks:**

---

#### Substance name

C14-C18 FAME Argent Energy - Fatty acids, C14-18 and C16-C18-unsatd., Me esters

### Identification of substance

---

#### Reference substance

Fatty acids, C14-18 and C16-18-unsatd., Me esters / UVCB substance, no IUPAC name available  
chemical name: C14-C18 and 16-C18 unsaturated alkyl carboxyl / 67762-26-9 / 267-007-0

#### EC number

267-007-0

#### EC name

EC Inventory

#### CAS number

67762-26-9

#### CAS name

Fatty acids, C14-18 and C16-C18-unsatd., Me esters

#### IUPAC name

UVCB substance, no IUPAC name available chemical name: C14-C18 and 16-C18 unsaturated alkyl carboxylic acids methyl esters. The substance is synthesised by transesterification of mixed animal fats (tallow, pig, chicken, beef origins) and vegetable oils (palm, soy, rape) with methanol to produce methylesters and glycerin or esterification of fatty acids to produce methyl esters and water.

### 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: Fatty acids, C14-18 and C16-C18-unsatd., Me esters

---

**UUID:** c6314f33-50cd-40ec-abc7-3ec117741ecb

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.298Z

**Remarks:**

---

## General Information

---

### Name

Fatty acids, C14-18 and C16-C18-unsatd., Me esters

### Type of composition

legal entity composition of the substance

### State / form

liquid

### Description

UVCB substance

Methods of manufacture of substance (migrated information):

1)Transesterification of natural oils with methanol to produce methylesters and glycerin.Temperature c.a 70°C

2)Separation in aqueous phase (glycerin and others) and FAME

## Degree of purity

---

EU: REACH

100

% (w/w)

## Constituents

---

### Reference substance

[Methyl decanoate / Methyl decanoate / 110-42-9 / 203-766-6](#)

#### EC number

203-766-6

#### EC name

EC Inventory

#### CAS number

110-42-9

#### CAS name

Decanoic acid, methyl ester

#### IUPAC name

Methyl decanoate

### Typical concentration

ca. 0.1

% (w/w)



**Concentration range**

>= 0                      < 2                      % (w/w)

## Reference substance

[methyl laurate](#) / [methyl laurate](#) / [111-82-0](#) / [203-911-3](#)

<b>EC number</b>	<b>EC name</b>
203-911-3	EC Inventory

CAS number	CAS name
111-82-0	

**IUPAC name**  
methyl laurate

### Typical concentration

< 0.1 % (w/w)

**Concentration range**

>= 0 < 2 % (w/w)

## Reference substance

methyl myristate / methyl myristate / 124-10-7 / 204-680-1

EC number	EC name
204-680-1	EC Inventory

CAS number	CAS name
124-10-7	

**IUPAC name**  
methyl myristate

### Typical concentration

ca. 2.5 % (w/w)

**Concentration range**

>= 2                      <= 8                      % (w/w)

## Reference substance

methyI palmitate / methyl palmitate / 112-39-0 / 203-966-3

<b>EC number</b>	<b>EC name</b>
203-966-3	EC Inventory

CAS number	CAS name
112-39-0	

**IUPAC name**  
methyl palmitate

**Typical concentration**

ca. 23.9 % (w/w)

**Concentration range**

>= 2 <= 62 % (w/w)

**Reference substance**

[methyl \(Z\)-hexadec-9-enoate / methyl hexadec-9-enoate / 1120-25-8 / 214-303-2](#)

**EC number**

214-303-2

**EC name**

EC Inventory

**CAS number**

1120-25-8

**CAS name****IUPAC name**

methyl hexadec-9-enoate

**Typical concentration**

ca. 2.9 % (w/w)

**Concentration range**

>= 2 <= 9 % (w/w)

**Reference substance**

[methyl stearate / methyl stearate / 112-61-8 / 203-990-4](#)

**EC number**

203-990-4

**EC name**

EC Inventory

**CAS number**

112-61-8

**CAS name****IUPAC name**

methyl stearate

**Typical concentration**

ca. 17.8 % (w/w)

**Concentration range**

>= 2 <= 28 % (w/w)

**Reference substance**

[methyl oleate / methyl octadec-9-enoate / 112-62-9 / 203-992-5](#)

**EC number**

203-992-5

**EC name**

EC Inventory

---

CAS number	CAS name
------------	----------

112-62-9

**IUPAC name**

methyl octadec-9-enoate

**Typical concentration**

ca. 41.9 % (w/w)

**Concentration range**

>= 13 <= 95 % (w/w)

**Reference substance**

[methyl linoleate](#) / [methyl octadeca-9,12-dienoate](#) / [112-63-0](#) / [203-993-0](#)

**EC number**

203-993-0

**EC name**

EC Inventory

**CAS number**

112-63-0

**CAS name**

**IUPAC name**

methyl octadeca-9,12-dienoate

**Typical concentration**

ca. 7.4 % (w/w)

**Concentration range**

>= 1 <= 40 % (w/w)

**Reference substance**

[methyl \(9Z,12Z,15Z\)-9,12,15-octadecatrienoate](#) / [methyl octadeca-9,12,15-trienoate](#) / [301-00-8](#) / [206-102-3](#)

**EC number**

206-102-3

**EC name**

EC Inventory

**CAS number**

301-00-8

**CAS name**

**IUPAC name**

methyl octadeca-9,12,15-trienoate

**Typical concentration**

ca. 2.1 % (w/w)

**Concentration range**

>= 1 <= 20 % (w/w)

**Reference substance**[methyl icosanoate](#) / [methyl icosanoate](#) / 1120-28-1 / 214-304-8**EC number**

214-304-8

**EC name**

EC Inventory

**CAS number**

1120-28-1

**CAS name****IUPAC name**

methyl icosanoate

**Typical concentration**

ca. 0.2 % (w/w)

**Concentration range**

&gt;= 0 &lt; 2 % (w/w)

**Reference substance**[methyl cis-icos-11-enoate](#) / [methyl icos-11-enoate](#) / 2390-09-2 / 219-226-8**EC number**

219-226-8

**EC name**

EC Inventory

**CAS number**

2390-09-2

**CAS name****IUPAC name**

methyl icos-11-enoate

**Typical concentration**

ca. 0.3 % (w/w)

**Concentration range**

&gt;= 0 &lt; 2 % (w/w)

**Reference substance**[methyl docosanoate](#) / [methyl docosanoate](#) / 929-77-1 / 213-207-8**EC number**

213-207-8

**EC name**

EC Inventory

**CAS number**

929-77-1

**CAS name****IUPAC name**

methyl docosanoate

**Typical concentration**

ca. 0.1 % (w/w)

**Concentration range**

>= 0 < 2 % (w/w)

**Reference substance**

[methyl \(Z\)-docos-13-enoate](#) / [methyl docos-13-enoate](#) / 1120-34-9 / 214-305-3

**EC number**

214-305-3

**EC name**

EC Inventory

**CAS number**

1120-34-9

**CAS name****IUPAC name**

methyl docos-13-enoate

**Typical concentration**

< 0.1 % (w/w)

**Concentration range**

>= 0 < 2 % (w/w)

**Reference substance**

[methyl tetracosanoate](#) / [methyl tetracosanoate](#) / 2442-49-1 / 219-475-2

**EC number**

219-475-2

**EC name**

EC Inventory

**CAS number**

2442-49-1

**CAS name****IUPAC name**

methyl tetracosanoate

**Typical concentration**

ca. 0.1 % (w/w)

**Concentration range**

>= 0 < 2 % (w/w)

**Reference substance**

[methyl \(Z\)-tetracos-15-enoate](#) / [methyl tetracos-15-enoate](#) / 2733-88-2 / 220-352-0

**EC number**

220-352-0

**EC name**

EC Inventory

**CAS number**

2733-88-2

**CAS name****IUPAC name**

methyl tetracos-15-enoate

---

**Typical concentration**

< 0.1 % (w/w)

**Concentration range**

>= 0 < 2 % (w/w)

**Reference substance**

[methanol / methanol / 67-56-1 / 200-659-6](#)

**EC number**

200-659-6

**EC name**

EC Inventory

**CAS number**

67-56-1

**CAS name**

methanol

**IUPAC name**

methanol

**Typical concentration**

< 0.01 % (w/w)

**Concentration range**

>= 0 < 0.2 % (w/w)

**Reference substance**

[Glycerol, monoglycerides, diglycerides, triglycerides of Fatty acids, C16-C18 and C18-unsatd. / Glycerol, monoglycerides, diglycerides, triglycerides of Fatty acids, C16-C18 and C18-unsatd.](#)

**EC number****EC name****CAS number****CAS name****IUPAC name**

Glycerol, monoglycerides, diglycerides, triglycerides of Fatty acids, C16-C18 and C18-unsatd.

**Typical concentration**

< 0.15 % (w/w)

**Concentration range**

>= 0 < 3.5 % (w/w)

---

**Characterisation of polymers**

---

**Reactive functional groups**

**Polymer contains only low concern reactive functional groups**

false

---

## Identifiers

### FLEXIBLE\_RECORD: Identifiers

---

**UUID:** de00cf7c-9452-44ff-879f-ecacf8a301ed

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.305Z

**Remarks:**

---

## Regulatory programme identifiers

---

### Regulatory programme identifiers

<b>Regulatory programme</b>
REACH registration number
<b>ID</b>
01-2119471662-36-0041
<b>Regulatory programme</b>
REACH inquiry number
<b>ID</b>
06-2120863235-54-0000

---

## Analytical Information

### FLEXIBLE\_RECORD: Analytical Information

---

**UUID:** b06f5cf1-7acb-4f87-8d49-85cb52b436c8

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.301Z

**Remarks:**

---

## Analytical information

---

EU: REACH

## Methods and results of analysis

---

### Analytical determination

**Purpose of analysis**

identification and quantification

**Analysis type**

gas chromatography

infrared spectroscopy

nuclear magnetic resonance

UV/Visible spectroscopy

**Type of information provided**

methods and results

**Attached methods/results**

Biodiesel - Report 184883.pdf / 1.517 MB (application/pdf)

**Remarks**

Analytical methods and spectral data:

GC, H1NMR, UV-Vis, IR were performed. The methods, experimental conditions and results are summarised in the report

### Optical activity

no

**Remarks**

Optical activity is not an expected property of the substance



---

## Suppliers

### FLEXIBLE\_RECORD: Supplier.001

---

**UUID:** 1d3bb3b2-cd3c-4c29-9e50-22cac7a0f26a

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.335Z

**Remarks:**

---

## Only representation information

---

### Assignment from non EU manufacturer

Stanlow transfer REACH reg.pdf / 125.944 KB (application/pdf)

---

## Assessment approach (assessment entities)

### FIXED\_RECORD: Assessment approach

---

**UUID:** 529818cb-e17e-4fc1-840b-d2dd337e5162

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.279Z

**Remarks:**

---

---

# Classification & Labelling and PBT assessment

## PBT assessment

### FLEXIBLE\_SUMMARY: PBT assessment.001

---

**UUID:** 386086d4-b68e-4fc3-b554-a6eb0a967330

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.353Z

**Remarks:**

---

## PBT assessment: overall result

---

### PBT status

the substance is not PBT / vPvB

### Justification

Fatty acids, C14-18 and C16-18-unsatd., Me esters is not regarded as P or vP based on ready biodegradability

Fatty acids, C14-18 and C16-18-unsatd., Me esters is not regarded as Bioaccumulative based on the measured BCF of 3 [Fina 1997]. It indicates that Fatty acids, C16-18 and C18-unsatd., Me esters does not significantly accumulate in organisms

Fatty acids, C14-18 and C16-18-unsatd., Me esters is not regarded as toxic according to Annex I to 67/548/EEC and the data on toxicity provided herein]. Fatty acids, C16-18 and C18-unsatd., Me esters is not regarded as carcinogenic (category 1 or 2), mutagenic (category 1 or 2) or toxic for reproduction (category 1, 2 or 3). There are no other evidence of chronic toxicity.

---

## Manufacture, use and exposure

### Estimated quantities

**FLEXIBLE\_RECORD: 2020**

---

**UUID:** f8e1f60f-ebd2-475b-88d8-17c1e2a6292a

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.332Z

**Remarks:**

---

**Year**

2020

**Total tonnage (tonnes / year)** \_\_\_\_\_

**Manufactured**

74223

**Imported**

0

---

**FLEXIBLE\_RECORD: 2019**

---

**UUID:** c3ec64dd-3606-49e8-bb51-06e3fc41868c

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.337Z

**Remarks:**

---

**Year**

2019

**Total tonnage (tonnes / year)** 

---

**Manufactured**

65494

---

**FLEXIBLE\_RECORD: 2018**

---

**UUID:** ad340abd-3bf9-42d0-8099-e117845c4f6a

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.346Z

**Remarks:**

---

**Year**

2018

**Total tonnage (tonnes / year)** 

---

**Manufactured**

67237

---

**FLEXIBLE\_RECORD: 2017**

---

**UUID:** 7b1e783b-4ae0-403a-8c48-ca5586151630

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.350Z

**Remarks:**

---

**Year**

2017

**Total tonnage (tonnes / year)** 

---

**Manufactured**

30743

---

## Information on mixtures

### FLEXIBLE\_RECORD: Biodiesel

---

**UUID:** 268c7cd6-322e-42a2-896b-9a95c78a4566

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.317Z

**Remarks:**

---

EU: REACH

**Trade name of mixture**

Biodiesel

**Type of mixture**

solution

**Typical concentration**

> 10                      <= 100                      % (w/w)



---

## Use and exposure information

### Formulation or re-packing

**FLEXIBLE\_RECORD:** Production of Biodiesel

---

**UUID:** 70f69f93-5efd-405c-baf8-c820a09e2396

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.322Z

**Remarks:**

---

## Formulation

---

**Use number**

2

**Use name**

Production of Biodiesel

**Contributing activity / technique for the environment**

**Environmental release category (ERC)**

ERC2: Formulation into mixture

**Contributing activity / technique for workers**

**Process category (PROC)**

PROC 5: Mixing or blending in batch processes

**Process category (PROC)**

PROC 8b: Transfer of substance or mixture (charging and discharging) at dedicated facilities

**Product category formulated**

PC 13: Fuels

**Technical function of the substance during formulation**

fuels and fuel additives

**Substance supplied to that use in form of**

as such

**Limited number of sites for this use**

false

---

## Widespread uses by professional workers

**FLEXIBLE\_RECORD:** Use of Biodiesel

---

**UUID:** 4a5ea7aa-f29a-40a8-92b6-50acff438da0

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.308Z

**Remarks:**

---

## Uses by professional workers

---

**Use number**

3

**Use name**

Use of Biodiesel

**Any precursor use(s)**

false

**Contributing activity / technique for the environment**

**Environmental release category (ERC)**

ERC9b: Widespread use of functional fluid (outdoor)

**Contributing activity / technique for workers**

**Process category (PROC)**

PROC 9: Transfer of substance or mixture into small containers (dedicated filling line, including weighing)

**Product category used**

PC 13: Fuels

**Technical function of the substance during use**

fuels and fuel additives

**Substance supplied to that use in form of**

in a mixture

**Subsequent service life relevant to this use**

no

**Total EU tonnage for this use**

false

## Use takes place under rigorously contained conditions

---

**Rigorously contained system with strict control for manual interventions**

false

**Rigorously contained system with minimisation of release to the environment**

false

---

## Guidance on safe use

### FLEXIBLE\_RECORD: Guidance on safe use

---

**UUID:** a4050ace-a862-475f-aac8-7bd3eb6208e1

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.304Z

**Remarks:**

---

## Administrative data

---

EU: REACH

## First-aid measures

---

### EYES

Irrigate eyes with a heavy stream of water for at least 15 to 20 minutes

### SKIN

Wash exposed areas of the body with soap and water

### INHALATION

Remove from area of exposure; seek medical attention if symptoms persist

### INGESTION

Give one or two glasses of water to drink. If gastro-intestinal symptoms develop, consult medical personnel. (Never give anything by mouth to an unconscious person)

## Fire-fighting measures

---

### EXTINGUISHING MEDIA:

Dry chemical, foam, halon (may not be permissible in some countries), CO<sub>2</sub>, water spray (fog). Water stream may splash the burning liquid and spread fire.

### SPECIAL FIRE FIGHTING PROCEDURES:

Use water spray to cool drums exposed to fire.

### UNUSUAL FIRE AND EXPLOSION HAZARDS:

Biodiesel soaked rags or spill absorbents (i.e. oil dry, polypropylene socks, sand, etc.) can cause spontaneous combustion if stored near combustibles and not handled properly. Store biodiesel soaked rags or spill absorbents in approved safety containers and dispose of properly. Oil soaked rags may be washed with soap and water and allowed to dry in well ventilated area. Firefighters should use self-contained breathing apparatus to avoid exposure to smoke and vapor

## Accidental release measures

---

Remove sources of ignition, contain spill to smallest area possible. Stop leak if possible.

Pick up small spills with absorbent materials and dispose of properly to avoid spontaneous combustion (see unusual fire and explosion hazards above).

---

Recover large spills for salvage or disposal. Wash hard surfaces with safety solvent or detergent to remove remaining oil film. Greasy nature will result in a slippery surface.

## Handling and storage

---

Store in closed containers between 50°F and 120°F.  
Keep away from oxidizing agents, excessive heat, and ignition sources.  
Store and use in well ventilated areas.  
Do not store or use near heat, spark, or flame, store out of sun.  
Do not puncture, drag, or slide this container.  
Drum is not a pressure vessel; never use pressure to empty.

## Transport information

---

### Land transport (UN RTDG/ADR/RID)

---

**UN number**  
Not classified

**Labels**  
Not classified

### Inland waterway transport (UN RTDG/ADN(R))

---

**UN number**  
Not classified

**Labels**  
Not classified

### Marine transport (UN RTDG/IMDG)

---

**UN number**  
Not classified

#### Shipping information

**Proper shipping name and description**  
Not classified

**Chemical name**  
Not classified

**Labels**  
Not classified

**Marine pollutant**  
false

### Air transport (UN RTDG/ICAO/IATA)

---

**UN number**  
Not classified

---

## Shipping information

### Proper shipping name and description

Not classified

### Chemical name

Not classified

## Labels

Not classified

## Exposure controls / personal protection

### RESPIRATORY PROTECTION:

If vapors or mists are generated, wear a NIOSH approved organic vapor/mist respirator.

### PROTECTIVE CLOTHING:

Safety glasses, goggles, or face shield recommended to protect eyes from mists or splashing. PVC coated gloves recommended to prevent skin contact.

### OTHER PROTECTIVE MEASURES:

Employees must practice good personal hygiene, washing exposed areas of skin several times daily and laundering contaminated clothing before re-use.

## Stability and reactivity

### GENERAL:

This product is stable and hazardous reaction will not occur.

### INCOMPATIBLE MATERIALS AND CONDITIONS TO AVOID:

Strong oxidizing agents. Strong basis. It reacts with strong basis to produce methanol

### HAZARDOUS DECOMPOSITION PRODUCTS:

Combustion produces carbon monoxide, carbon dioxide along with thick smoke.

## Disposal considerations

### WASTE DISPOSAL

Dispose in a safe manner in accordance with local/national regulations

---

## Assessment reports

### Chemical Safety Report (CSR)

**FLEXIBLE\_RECORD: CSR ARGENT ENERGY**

---

**UUID:** 782bdd13-bd5a-4139-b9b5-07d159567db4

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.328Z

**Remarks:**

---

### Administrative data

---

EU: REACH

### Chemical Safety Report (CSR)

---

**Type of CSR**

Joint CSR (joint uses)

**CSR contains**

Part A

Part B section 1 to 8

Part B section 9 and 10

**Chemical safety assessment/report tool used**

Chesar

**Chemical safety report (CSR)**

FAME\_CSR\_20Feb2021.pdf / 1.306 MB (application/pdf)

---

# References

## REFERENCE\_SUBSTANCE: Fatty acids, C14-18 and C16-18-unsatd., Me esters

---

**UUID:** cc0c7ecd-4124-4fa6-8345-fe6211124dda

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.223Z

**Remarks:**

---

### Reference substance name

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

### IUPAC name

UVCB substance, no IUPAC name available chemical name: C14-C18 and 16-C18 unsaturated alkyl carboxylic acids methyl esters. The substance is synthesised by transesterification of mixed animal fats (tallow, pig, chicken, beef origins) and vegetable oils (palm, soy, rape) with methanol to produce methylesters and glycerin or esterification of fatty acids to produce methyl esters and water.

### Description

This substance is identified by SDA Substance Name: C14-C18 and 16-C18 unsaturated alkyl carboxylic acid methyl ester and SDA Reporting Number: 04-010-00. The following other substances from the EC inventory will fall within the same description: Fatty acids, rape-oil, me esters - EINECS 287-828-8 - CAS 85586-25-0 Fatty acids, tallow, Me esters - EINECS 262-989-7 - CAS 61788-61-2 Tallow, Me esters - EINECS 272-743-0 - CAS 68910-48-5 The substance is synthesised by transesterification of mixed animal fats (tallow, pig, chicken, beef origins) and vegetable oils (palm, soy, rape) with methanol to produce methylesters and glycerin or esterification of fatty acids to produce methyl esters and water. In this description enter all substances generated by natural oils with fatty acid chains length focused on C14 - C18 and C16 - C18 unsatd., above 2%. Example of such vegetable raw materials are rape oil, Tallow oil, and all analogous derivatives, except from jatropha oil, due to its toxicity. Example of animal raw material is the beef fat. A threshold of 2% has been chosen to consider Alkyl Chain Fatty Acid within the name of the substance following the rules stated in the "Addendum III of the TCSA inventory 1978". It has also to be taken into account the Test method tolerances and repeatability/reproducibility: measuring ester content using EN14103 gives a repeatability (r) figure of 1.6 and a reproducibility (R) of 3.1. (ASG infoletter: Tolerance in analytic test methods); Further details are in the documents of justification of the naming and the category

## Inventory

---

### Inventory number

#### Inventory name

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

#### Inventory

EC Inventory

#### Inventory number

267-007-0

#### CAS number

67762-26-9

---

**Molecular formula****Description**

This substance is identified by SDA Substance Name: C14-C18 and C16-C18 unsaturated alkyl carboxylic acid methyl ester and SDA Reporting Number: 04-010-00.

**CAS number**

67762-26-9

**CAS name**

Fatty acids, C14-18 and C16-C18-unsatd., Me esters

---

**Molecular and structural information****Molecular formula**

UVCB substance, not univocal molecular formula available

**Molecular weight**

ca. 290

**SMILES notation**

UVCB substance, not univocal SMILE notation available

**InChI**

UVCB substance, not univocal InChI notation available

**Remarks**

UVCB substance, not univocal structural formula formula available

---

**Related substances****Identifier**

CAS name

**Identity**

Fatty acids, rape oil, Me esters

**Relation**

other:

**Identifier**

CAS number

**Identity**

85586-25-0

**Relation**

other:

**Identifier**

CAS name

**Identity**

Fatty acids, tallow, Me esters

**Relation**

other:



---

<b>Identifier</b> CAS number
<b>Identity</b> 61788-61-2
<b>Relation</b> other:
<b>Identifier</b> CAS name
<b>Identity</b> Tallow, me esters
<b>Identifier</b> CAS number
<b>Identity</b> 68910-48-5

**Group / category information**  
Fatty Acid Methyl Esters Category

---

# REFERENCE\_SUBSTANCE: Glycerol, monoglycerides, diglycerides, triglycerides of Fatty acids, C16-C18 and C18-unsatd.

---

**UUID:** 9d56924b-471b-465f-89cc-fcce950cba4a

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.227Z

**Remarks:**

---

## Reference substance name

Glycerol, monoglycerides, diglycerides, triglycerides of Fatty acids, C16-C18 and C18-unsatd.

## IUPAC name

Glycerol, monoglycerides, diglycerides, triglycerides of Fatty acids, C16-C18 and C18-unsatd.

## Description

Small Residues of starting material and partially reacted material

## Inventory

---

### No inventory information available - Justification

not applicable

## Molecular and structural information

---

### Molecular formula

Not applicable

### SMILES notation

Not applicable

### InChI

Not applicable

### Remarks

A singular structural formula is not possible for this substance

---

# REFERENCE\_SUBSTANCE: methanol

---

**UUID:** ECB5-22d9884a-cae8-411d-8d6d-dcece832d4b2

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.227Z

**Remarks:**

---

EU: CLP, EU: REACH

**Reference substance name**

methanol

**IUPAC name**

methanol

## Inventory

---

**Inventory number**

**Inventory name**

methanol

**Inventory**

EC Inventory

**Inventory number**

200-659-6

**CAS number**

67-56-1

**Molecular formula**

CH<sub>4</sub>O

**Description**

**CAS number**

67-56-1

**CAS name**

methanol

## Synonyms

---

**Synonyms**

**Identity**

Methanol

**Identity**

Methanol

## Molecular and structural information

---

---

EU: CLP, EU: REACH

**Molecular formula**

CH<sub>4</sub>O

**Molecular weight**

32.0419

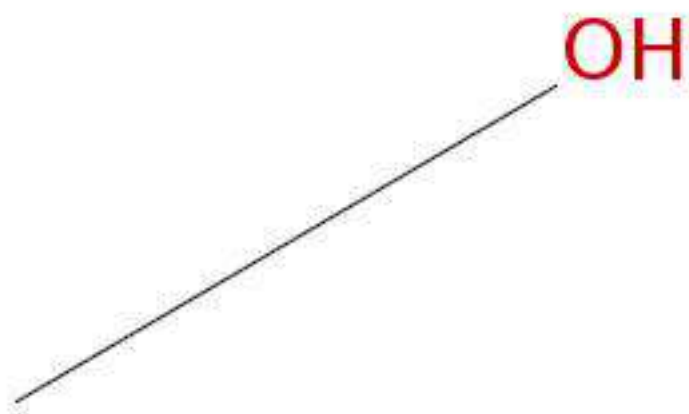
**SMILES notation**

CO

**InChI**

InChI=1/CH<sub>4</sub>O/c1-2/h2H,1H3

**Structural formula**



---

**Related substances**

**Group / category information**

DSL Category: Organics

---

# REFERENCE\_SUBSTANCE: methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate

---

**UUID:** ECB5-334b122a-96e7-41eb-9078-f5a8ac1676ee

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

## Reference substance name

methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate

## IUPAC name

methyl octadeca-9,12,15-trienoate

## Inventory

---

### Inventory number

**Inventory name**

methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate

**Inventory**

EC Inventory

**Inventory number**

206-102-3

**CAS number**

301-00-8

**Molecular formula**

C<sub>19</sub>H<sub>32</sub>O<sub>2</sub>

**Description****CAS number**

301-00-8

## Synonyms

---

### Synonyms

**Identity**

9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-

**Identity**

9,12,15-Octadecatrienoic acid, methyl ester, (9Z,12Z,15Z)-

## Molecular and structural information

---

**Molecular formula**

C<sub>19</sub>H<sub>32</sub>O<sub>2</sub>

---

---

**Molecular weight**

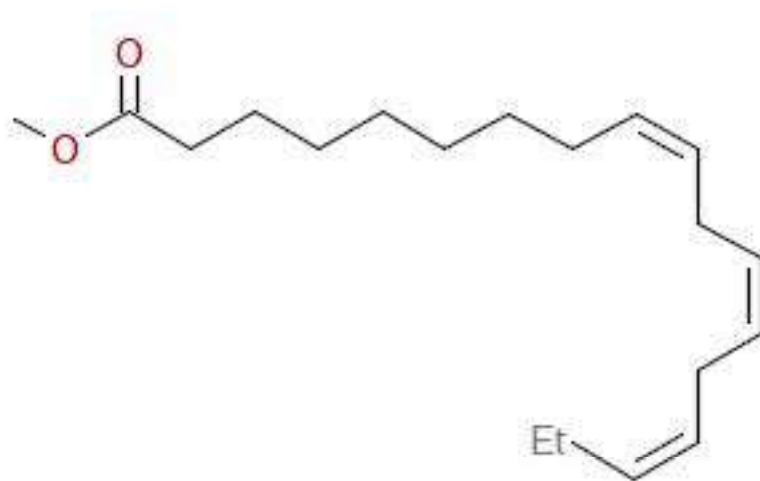
292.4562

**SMILES notation**

CC\C=C/C\C=C/C\C=C/CCCCCCCC(=O)OC

**InChI**

InChI=1/C19H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h4-5,7-8,10-11H,3,6,9,12-18H2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

DSL Category: Organics

---

# REFERENCE\_SUBSTANCE: methyl (Z)-docos-13-enoate

---

**UUID:** ECB5-4a39484d-9ac5-47c6-9e80-ed5b8e68767e

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.226Z

**Remarks:**

---

**Reference substance name**

methyl (Z)-docos-13-enoate

**IUPAC name**

methyl docos-13-enoate

## Inventory

---

**Inventory number**

**Inventory name**

methyl (Z)-docos-13-enoate

**Inventory**

EC Inventory

**Inventory number**

214-305-3

**CAS number**

1120-34-9

**Molecular formula**

C<sub>23</sub>H<sub>44</sub>O<sub>2</sub>

**Description**

**CAS number**

1120-34-9

## Synonyms

---

**Synonyms**

**Identity**

13-Docosenoic acid, methyl ester, (Z)-

**Identity**

13-Docosenoic acid, methyl ester, (13Z)-

## Molecular and structural information

---

**Molecular formula**

C<sub>23</sub>H<sub>44</sub>O<sub>2</sub>

---

---

**Molecular weight**

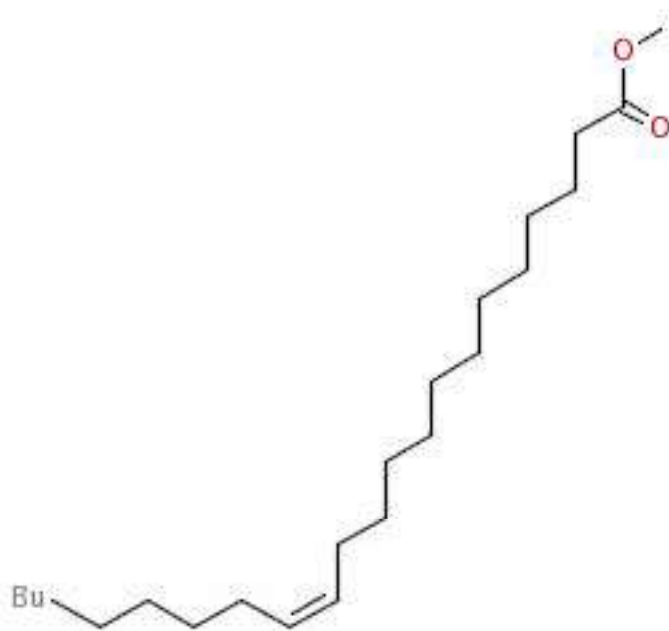
352.5943

**SMILES notation**

CCCCCCCC\C=C/CCCCCCCCCCCCC(=O)OC

**InChI**

InChI=1/C23H44O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)25-2/h10-11  
H,3-9,12-22H2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

USEPA Category: Esters



---

# REFERENCE\_SUBSTANCE: methyl (Z)-hexadec-9-enoate

---

**UUID:** ECB5-61798f8c-ecde-4594-819b-badc7f0dbf5a

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

**Reference substance name**

methyl (Z)-hexadec-9-enoate

**IUPAC name**

methyl hexadec-9-enoate

## Inventory

---

**Inventory number**

**Inventory name**

methyl (Z)-hexadec-9-enoate

**Inventory**

EC Inventory

**Inventory number**

214-303-2

**CAS number**

1120-25-8

**Molecular formula**

C<sub>17</sub>H<sub>32</sub>O<sub>2</sub>

**Description**

**CAS number**

1120-25-8

## Synonyms

---

**Synonyms**

**Identity**

9-HEXADECENOIC ACID, METHYL ESTER, (Z)-

## Molecular and structural information

---

**Molecular formula**

C<sub>17</sub>H<sub>32</sub>O<sub>2</sub>

**Molecular weight**

268.4348

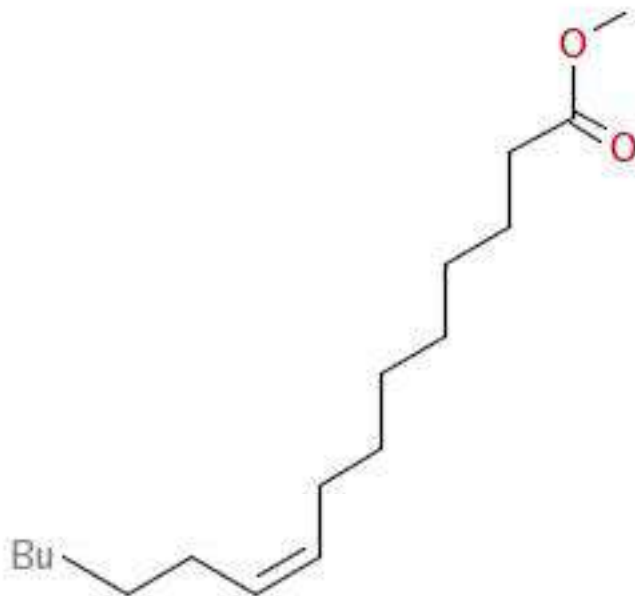
---

**SMILES notation**

CCCCC\C=C/CCCCCCCC(=O)OC

**InChI**

InChI=1/C17H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19-2/h8-9H,3-7,10-16H2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

USEPA Category: Esters;Esters (Chronic toxicity)

---

# REFERENCE\_SUBSTANCE: methyl (Z)-tetracos-15-enoate

---

**UUID:** ECB5-1f1e4046-16ad-488e-8929-6a01300a293c

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.226Z

**Remarks:**

---

**Reference substance name**  
methyl (Z)-tetracos-15-enoate

**IUPAC name**  
methyl tetracos-15-enoate

## Inventory

---

### Inventory number

**Inventory name**  
methyl (Z)-tetracos-15-enoate

**Inventory**  
EC Inventory

**Inventory number**  
220-352-0

**CAS number**  
2733-88-2

**Molecular formula**  
C<sub>25</sub>H<sub>48</sub>O<sub>2</sub>

**Description**

**CAS number**  
2733-88-2

## Synonyms

---

### Synonyms

**Identity**  
15-Tetracosenoic acid, methyl ester, (Z)-

## Molecular and structural information

---

**Molecular formula**  
C<sub>25</sub>H<sub>48</sub>O<sub>2</sub>

**Molecular weight**

380.6474

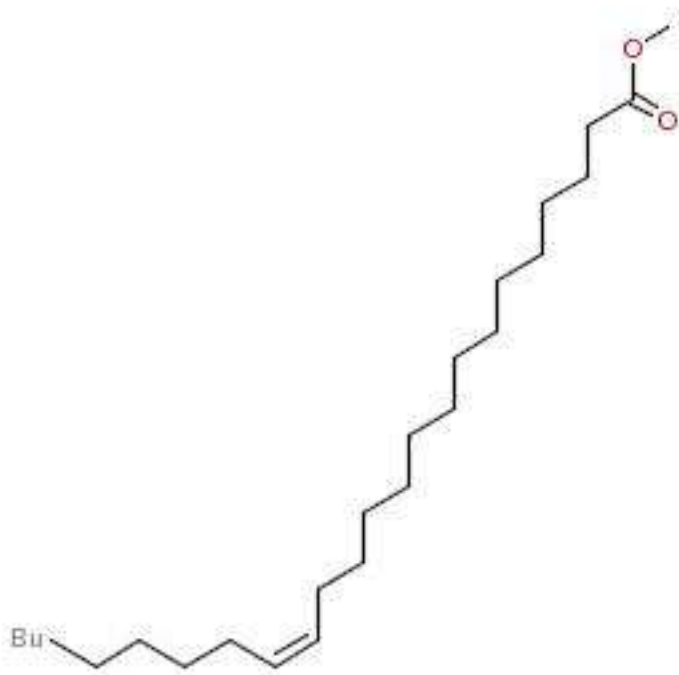
---

**SMILES notation**

CCCCCCCCC=C/CCCCCCCCCCCCC(=O)OC

**InChI**

InChI=1/C25H48O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25(26)27-2/h10-11H,3-9,12-24H2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

USEPA Category: Esters

---

# REFERENCE\_SUBSTANCE: methyl cis-icos-11-enoate

---

**UUID:** ECB5-c8fe7d4f-f489-41a6-be77-28082a38d74d

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.226Z

**Remarks:**

---

**Reference substance name**

methyl cis-icos-11-enoate

**IUPAC name**

methyl icos-11-enoate

## Inventory

---

**Inventory number**

**Inventory name**

methyl cis-icos-11-enoate

**Inventory**

EC Inventory

**Inventory number**

219-226-8

**CAS number**

2390-09-2

**Molecular formula**

C<sub>21</sub>H<sub>40</sub>O<sub>2</sub>

**Description**

**CAS number**

2390-09-2

## Synonyms

---

**Synonyms**

**Identity**

11-Eicosenoic acid, methyl ester, (Z)-

## Molecular and structural information

---

**Molecular formula**

C<sub>21</sub>H<sub>40</sub>O<sub>2</sub>

**Molecular weight**

324.5411

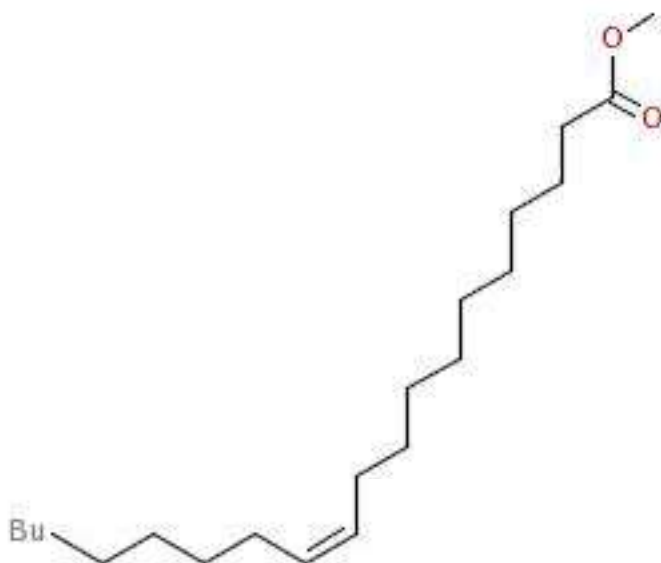
---

**SMILES notation**

CCCCCCCCC=C/CCCCCCCCC(=O)OC

**InChI**

InChI=1/C21H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h10-11H,3-9,12-20H2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

USEPA Category: Esters

---

# REFERENCE\_SUBSTANCE: Methyl decanoate

---

**UUID:** 3d088e09-7639-4f6e-b92b-1bd5b8c50d57

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

## Reference substance name

Methyl decanoate

## IUPAC name

Methyl decanoate

## Inventory

---

### Inventory number

#### Inventory name

methyl decanoate

#### Inventory

EC Inventory

#### Inventory number

203-766-6

#### CAS number

110-42-9

#### Molecular formula

C<sub>11</sub>H<sub>22</sub>O<sub>2</sub>

#### Description

### CAS number

110-42-9

### CAS name

Decanoic acid, methyl ester

## Molecular and structural information

---

### Molecular formula

C<sub>11</sub>H<sub>22</sub>O<sub>2</sub>

### Molecular weight

ca. 186.29

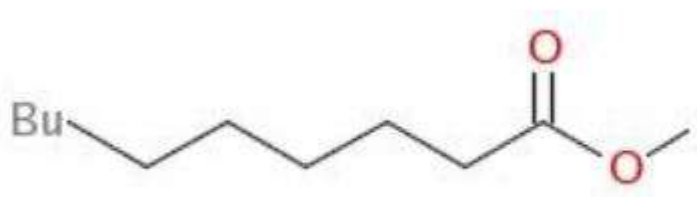
### SMILES notation

O=C(CCCCCCCCC)OC

---

**InChI**

1/C11H22O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3-10H2,1-2H3

**Structural formula**



---

# REFERENCE\_SUBSTANCE: methyl docosanoate

---

**UUID:** ECB5-525c3f91-f83b-4b7a-8dc7-00f45f3e8534

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.226Z

**Remarks:**

---

## Reference substance name

methyl docosanoate

## IUPAC name

methyl docosanoate

## Inventory

---

### Inventory number

**Inventory name**

methyl docosanoate

**Inventory**

EC Inventory

**Inventory number**

213-207-8

**CAS number**

929-77-1

**Molecular formula**

C<sub>23</sub>H<sub>46</sub>O<sub>2</sub>

**Description****CAS number**

929-77-1

## Synonyms

---

### Synonyms

**Identity**

Docosanoic acid, methyl ester

**Identity**

Docosanoic acid, methyl ester

## Molecular and structural information

---

**Molecular formula**

C<sub>23</sub>H<sub>46</sub>O<sub>2</sub>

---

**Molecular weight**

354.6101

**SMILES notation**

CCCCCCCCCCCCCCCCCCCC(=O)OC

**InChI**

InChI=1/C23H46O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)25-2/h3-22H  
2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

USEPA Category: Esters

---

# REFERENCE\_SUBSTANCE: methyl icosanoate

---

**UUID:** ECB5-bd93be9a-16e5-47ef-a531-ccabb6985fbe

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.226Z

**Remarks:**

---

## Reference substance name

methyl icosanoate

## IUPAC name

methyl icosanoate

## Inventory

---

### Inventory number

**Inventory name**

methyl icosanoate

**Inventory**

EC Inventory

**Inventory number**

214-304-8

**CAS number**

1120-28-1

**Molecular formula**

C<sub>21</sub>H<sub>42</sub>O<sub>2</sub>

**Description****CAS number**

1120-28-1

## Synonyms

---

### Synonyms

**Identity**

Eicosanoic acid, methyl ester

**Identity**

Eicosanoic acid, methyl ester

## Molecular and structural information

---

**Molecular formula**

C<sub>21</sub>H<sub>42</sub>O<sub>2</sub>

---

---

**Molecular weight**

326.557

**SMILES notation**

CCCCCCCCCCCCCCCCCCCC(=O)OC

**InChI**

InChI=1/C21H42O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-2/h3-20H2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

USEPA Category: Esters

---

# REFERENCE\_SUBSTANCE: methyl laurate

---

**UUID:** ECB5-4660b97a-3eb6-4677-a047-19a62db07da9

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

## Reference substance name

methyl laurate

## IUPAC name

methyl laurate

## Inventory

---

### Inventory number

**Inventory name**

methyl laurate

**Inventory**

EC Inventory

**Inventory number**

203-911-3

**CAS number**

111-82-0

**Molecular formula**

C<sub>13</sub>H<sub>26</sub>O<sub>2</sub>

**Description****CAS number**

111-82-0

## Synonyms

---

### Synonyms

**Identity**

Dodecanoic acid, methyl ester

**Identity**

Dodecanoic acid, methyl ester

**Identity**

Dodecanoic acid, methyl ester

## Molecular and structural information

---

---

**Molecular formula**

C<sub>13</sub>H<sub>26</sub>O<sub>2</sub>

**Molecular weight**

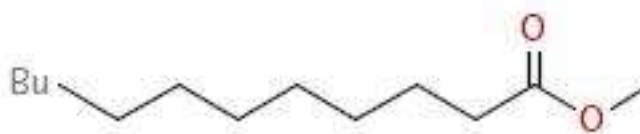
214.3443

**SMILES notation**

CCCCCCCCCCCC(=O)OC

**InChI**

InChI=1/C<sub>13</sub>H<sub>26</sub>O<sub>2</sub>/c1-3-4-5-6-7-8-9-10-11-12-13(14)15-2/h3-12H<sub>2</sub>,1-2H<sub>3</sub>

**Structural formula**

---

**Related substances****Group / category information**

DSL Category: Organics

USEPA Category: Esters;Esters (Chronic toxicity)

---

# REFERENCE\_SUBSTANCE: methyl linoleate

---

**UUID:** ECB5-403b9d75-31ce-49d8-85f7-f16987b8f4ab

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

## Reference substance name

methyl linoleate

## IUPAC name

methyl octadeca-9,12-dienoate

---

## Inventory

### Inventory number

**Inventory name**

methyl linoleate

**Inventory**

EC Inventory

**Inventory number**

203-993-0

**CAS number**

112-63-0

**Molecular formula**

C<sub>19</sub>H<sub>34</sub>O<sub>2</sub>

**Description****CAS number**

112-63-0

---

## Synonyms

### Synonyms

**Identity**

9,12-Octadecadienoic acid (Z,Z)-, methyl ester

**Identity**

9,12-Octadecadienoic acid (9Z,12Z)-, methyl ester

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## Molecular and structural information

**Molecular formula**

C<sub>19</sub>H<sub>34</sub>O<sub>2</sub>

---

**Molecular weight**

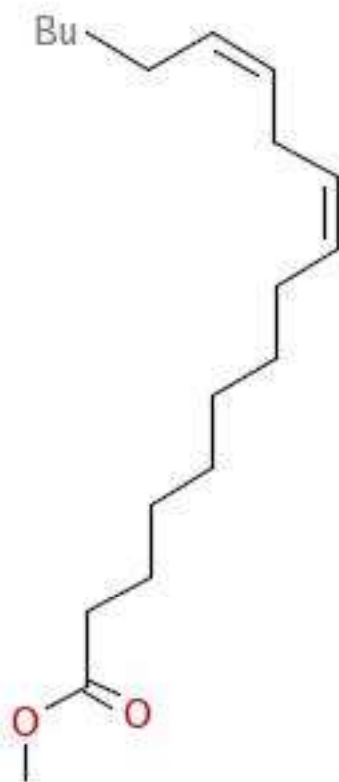
294.4721

**SMILES notation**

CCCCC\C=C/C\C=C/CCCCCCCC(=O)OC

**InChI**

InChI=1/C19H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h7-8,10-11H,3-6,9,12-18H2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

DSL Category: Organics



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# REFERENCE\_SUBSTANCE: methyl myristate

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**UUID:** ECB5-da256c7c-bbd3-445f-852d-a85805e6b457

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

## Reference substance name

methyl myristate

## IUPAC name

methyl myristate

---

## Inventory

### Inventory number

**Inventory name**

methyl myristate

**Inventory**

EC Inventory

**Inventory number**

204-680-1

**CAS number**

124-10-7

**Molecular formula**

C<sub>15</sub>H<sub>30</sub>O<sub>2</sub>

**Description****CAS number**

124-10-7

---

## Synonyms

### Synonyms

**Identity**

Myristic acid, methyl ester

**Identity**

Tetradecanoic acid, methyl ester

**Identity**

Tetradecanoic acid, methyl ester

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## Molecular and structural information

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**Molecular formula**

C<sub>15</sub>H<sub>30</sub>O<sub>2</sub>

**Molecular weight**

242.3975

**SMILES notation**

CCCCCCCCCCCCC(=O)OC

**InChI**

InChI=1/C<sub>15</sub>H<sub>30</sub>O<sub>2</sub>/c1-3-4-5-6-7-8-9-10-11-12-13-14-15(16)17-2/h3-14H<sub>2</sub>,1-2H<sub>3</sub>

**Structural formula**

---

**Related substances****Group / category information**

DSL Category: Organics

USEPA Category: Esters;Esters (Chronic toxicity)

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# REFERENCE\_SUBSTANCE: methyl oleate

---

**UUID:** ECB5-e2349b15-4d0c-49b0-8b77-8d410d710bca

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

## Reference substance name

methyl oleate

## IUPAC name

methyl octadec-9-enoate

---

## Inventory

### Inventory number

**Inventory name**

methyl oleate

**Inventory**

EC Inventory

**Inventory number**

203-992-5

**CAS number**

112-62-9

**Molecular formula**

C<sub>19</sub>H<sub>36</sub>O<sub>2</sub>

**Description****CAS number**

112-62-9

---

## Synonyms

### Synonyms

**Identity**

9-Octadecenoic acid (Z)-, methyl ester

**Identity**

9-Octadecenoic acid (9Z)-, methyl ester

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## Molecular and structural information

**Molecular formula**

C<sub>19</sub>H<sub>36</sub>O<sub>2</sub>

---

**Molecular weight**

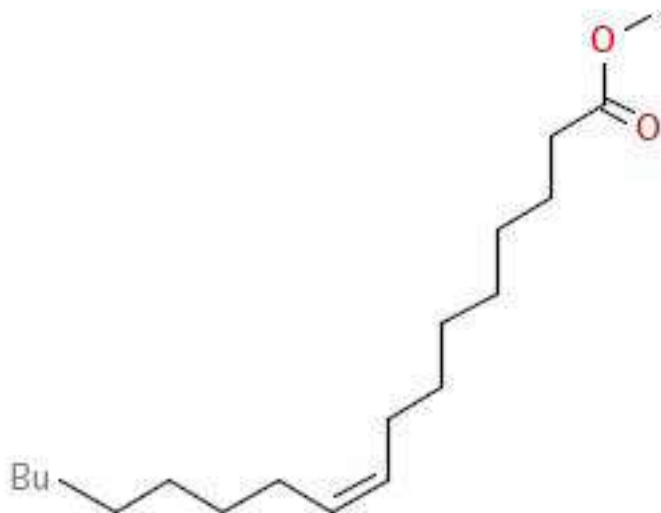
296.4879

**SMILES notation**

CCCCCCCC\C=C/CCCCCCCC(=O)OC

**InChI**

InChI=1/C19H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h10-11H,3-9,12-18H 2,1-2H3

**Structural formula**

---

**Related substances****Group / category information**

DSL Category: Organics

---

# REFERENCE\_SUBSTANCE: methyl palmitate

---

**UUID:** ECB5-49e6afa6-d9e0-468e-9e82-f12d598a45ca

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

## Reference substance name

methyl palmitate

## IUPAC name

methyl palmitate

## Inventory

---

### Inventory number

**Inventory name**

methyl palmitate

**Inventory**

EC Inventory

**Inventory number**

203-966-3

**CAS number**

112-39-0

**Molecular formula**

C<sub>17</sub>H<sub>34</sub>O<sub>2</sub>

**Description****CAS number**

112-39-0

## Synonyms

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### Synonyms

**Identity**

Hexadecanoic acid, methyl ester

**Identity**

Hexadecanoic acid, methyl ester

**Identity**

Hexadecanoic acid, methyl ester

## Molecular and structural information

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**Molecular formula**

C<sub>17</sub>H<sub>34</sub>O<sub>2</sub>

**Molecular weight**

270.4507

**SMILES notation**

CCCCCCCCCCCCCCCC(=O)OC

**InChI**

InChI=1/C<sub>17</sub>H<sub>34</sub>O<sub>2</sub>/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19-2/h3-16H<sub>2</sub>,1-2H<sub>3</sub>

**Structural formula**

---

**Related substances****Group / category information**

DSL Category: Organics

USEPA Category: Esters;Esters (Chronic toxicity)

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# REFERENCE\_SUBSTANCE: methyl stearate

---

**UUID:** ECB5-8632ca90-2141-4a6a-9b5f-93a0b25be88f

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.225Z

**Remarks:**

---

## Reference substance name

methyl stearate

## IUPAC name

methyl stearate

---

## Inventory

### Inventory number

**Inventory name**

methyl stearate

**Inventory**

EC Inventory

**Inventory number**

203-990-4

**CAS number**

112-61-8

**Molecular formula**

C<sub>19</sub>H<sub>38</sub>O<sub>2</sub>

**Description****CAS number**

112-61-8

---

## Synonyms

### Synonyms

**Identity**

Octadecanoic acid, methyl ester

**Identity**

Octadecanoic acid, methyl ester

**Identity**

Octadecanoic acid, methyl ester

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## Molecular and structural information

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**Molecular formula**

C<sub>19</sub>H<sub>38</sub>O<sub>2</sub>

**Molecular weight**

298.5038

**SMILES notation**

CCCCCCCCCCCCCCCCC(=O)OC

**InChI**

InChI=1/C<sub>19</sub>H<sub>38</sub>O<sub>2</sub>/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h3-18H<sub>2</sub>,1-2H<sub>3</sub>

**Structural formula**

---

**Related substances****Group / category information**

DSL Category: Organics

USEPA Category: Esters



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# REFERENCE\_SUBSTANCE: methyl tetracosanoate

---

**UUID:** ECB5-ae66fde0-d926-476d-8038-01ce33b7e9bf

**Dossier UUID:** 2018ab15-f003-4164-8bde-b46a3703478f

**Author:** Carol\_Sneddon

**Date:** 2021-03-04T20:54:12.226Z

**Remarks:**

---

## Reference substance name

methyl tetracosanoate

## IUPAC name

methyl tetracosanoate

## Inventory

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### Inventory number

**Inventory name**

methyl tetracosanoate

**Inventory**

EC Inventory

**Inventory number**

219-475-2

**CAS number**

2442-49-1

**Molecular formula**

C<sub>25</sub>H<sub>50</sub>O<sub>2</sub>

**Description****CAS number**

2442-49-1

## Synonyms

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### Synonyms

**Identity**

methyl\_tetracosanoate

## Molecular and structural information

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**Molecular formula**

C<sub>25</sub>H<sub>50</sub>O<sub>2</sub>

**Molecular weight**

382.6633

CCCCCCCCCCCCCCCCCC(=O)OC

InChI=1/C25H50O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25(26)27-2/h3-24H2,1-2H3

COC(=O)CCCCCCCCCCCCCCCCCCCI

## Related substances

USEPA Category: Esters