

**COVID-19 is an emerging, rapidly evolving situation.**Get the latest public health information from CDC: <https://www.coronavirus.gov>.Get the latest research from NIH: <https://www.nih.gov/coronavirus>.

## COMPOUND SUMMARY

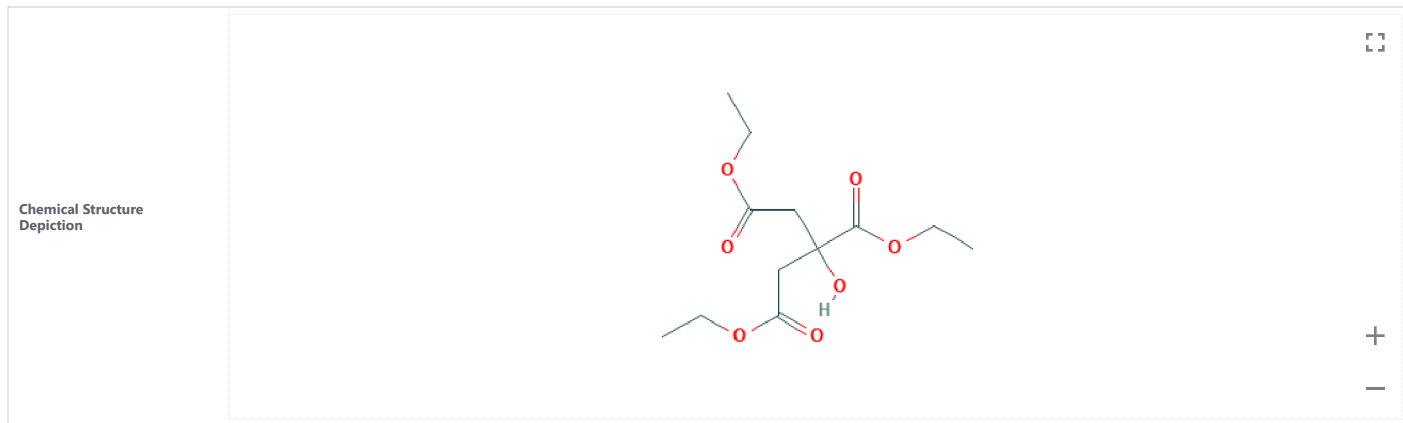
# Triethyl citrate

PubChem CID	6506				
Structure	  <p>2D                      3D</p> <p><a href="#">Find Similar Structures</a></p>				
Chemical Safety	 <p>Irritant</p> <p><a href="#">Laboratory Chemical Safety Summary (LCSS) Datasheet</a></p>				
Molecular Formula	$C_{12}H_{20}O_7$ or $(CH_2COOC_2H_5)_2COHCOOC_2H_5$				
Synonyms	TRIETHYL CITRATE 77-93-0 Ethyl citrate Citroflex 2 Eudraflex <input type="button" value="More..."/>				
Molecular Weight	276.28 g/mol				
Dates	<table> <tr> <td>Modify</td> <td>Create</td> </tr> <tr> <td>2020-12-26</td> <td>2005-03-26</td> </tr> </table>	Modify	Create	2020-12-26	2005-03-26
Modify	Create				
2020-12-26	2005-03-26				

## 1 Structures



### 1.1 2D Structure



### 1.2 3D Conformer



▶ PubChem

## 2 Names and Identifiers

### 2.1 Computed Descriptors

#### 2.1.1 IUPAC Name

triethyl 2-hydroxypropane-1,2,3-tricarboxylate

*Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)*

[▶ PubChem](#)

#### 2.1.2 InChI

InChI=1S/C12H20O7/c1-4-17-9(13)7-12(16,11(15)19-6-3)8-10(14)18-5-2/h16H,4-8H2,1-3H3

*Computed by InChI 1.0.5 (PubChem release 2019.06.18)*

[▶ PubChem](#)

#### 2.1.3 InChI Key

DOOTYTYQINUNNV-UHFFFAOYSA-N

*Computed by InChI 1.0.5 (PubChem release 2019.06.18)*

[▶ PubChem](#)

#### 2.1.4 Canonical SMILES

CCOC(=O)CC(CC(=O)OCC)(C(=O)OCC)O

*Computed by OEChem 2.1.5 (PubChem release 2019.06.18)*

[▶ PubChem](#)

## 2.2 Molecular Formula

C12H20O7

[▶ EU Food Improvement Agents; PubChem](#)

C12H20O7

(CH2COOC2H5)2COHCOOC2H5

[▶ ILO International Chemical Safety Cards \(ICSC\)](#)

## 2.3 Other Identifiers

### 2.3.1 CAS

77-93-0

[▶ ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency \(ECHA\); Hazardous Substances Data Bank \(HSDB\); Human Metabolome Database \(HMDB\); ILO International Chemical Safety Cards \(ICSC\)](#)

### 2.3.2 European Community (EC) Number

201-070-7

[▶ EU Food Improvement Agents; European Chemicals Agency \(ECHA\)](#)

### 2.3.3 ICSC Number

1350

[▶ ILO International Chemical Safety Cards \(ICSC\)](#)

### 2.3.4 NSC Number

8907

[▶ DTP/NCI](#)

### 2.3.5 RTECS Number

GE8050000

[▶ The National Institute for Occupational Safety and Health \(NIOSH\)](#)

## 2.3.6 UNII



8Z96QXD6UM

[▶ FDA/SPL Indexing Data](#)

## 2.3.7 JECFA Number



629

[▶ Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

## 2.3.8 FEMA Number



3083

[▶ Flavor and Extract Manufacturers Association \(FEMA\); Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

## 2.3.9 DSSTox Substance ID



DTXSID0040701

[▶ EPA DSSTox](#)

## 2.3.10 Wikipedia



Triethyl citrate

[▶ Wikipedia](#)

## 2.4 Synonyms



## 2.4.1 MeSH Entry Terms

ethyl citrate  
triethyl citrate[▶ MeSH](#)

## 2.4.2 Depositor-Supplied Synonyms



TRIETHYL CITRATE	Triaethylcitrat [German]	Triethyl 2-hydroxy-1,2,3-propanetricarboxylate	Triethyl Citrate, FCC	CTK319875
77-93-0	Crodamol TC	BRN 1801199	ACMC-1BFGJ	FEMA 3083
Ethyl citrate	Uniflex TEC	<b>8Z96QXD6UM</b>	EC 201-070-7	KS-00000W
Citroflex 2	UNII- <b>8Z96QXD6UM</b>	Triethylester kyseliny citronove [Czech]	DSSTox_CID_20701	WLN: 2OV1:
Eudraflex	NSC 8907	A13-00659	DSSTox_RID_79552	NSC8907
Hydragen CAT	Uniplex 80	2-Hydroxy-1,2,3-propanetricarboxylic acid, triethyl ester	DSSTox_GSID_40701	NSC-8907
Citric acid, triethyl ester	Hydagen C.A.T	E1505	SCHEMBL23465	ZINC164832
1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester	FEMA No. 3083	Triethyl citrate, 99%	KSC489Q7L	Tox21_30001
Triaethylcitrat	HSDB 729	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, 1,2,3-triethyl ester	Triethyl citrate 77-93-0	ANW-37130
Citric Acid Triethyl Ester	Triethyl citrate (NF)	TEC	CHEMBL464988	MFCD00005
triethyl 2-hydroxypropane-1,2,3-tricarboxylate	Triethyl citrate [NF]	2-Hydroxy-1,2,3-propanetricarboxylic acid, delta triethyl ester	1,2,3-triethyl 2-hydroxypropane-1,2,3-tricarboxylate	s6223
Triethylester kyseliny citronove	EINECS 201-070-7	Citric acid triethyl	DTXSID0040701	Triethyl citr:

[▶ PubChem](#)

## 3 Chemical and Physical Properties



### 3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	276.28 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
XLogP3-AA	0.1	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	7	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	11	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	276.120903 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Monoisotopic Mass	276.120903 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Topological Polar Surface Area	99.1 Å <sup>2</sup>	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	19	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	304	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2019.01.04)

► [PubChem](#)

## 3.2 Experimental Properties



### 3.2.1 Physical Description



Liquid

► [EPA Chemicals under the TSCA](#)

Odourless, practically colourless, oily liquid

► [EU Food Improvement Agents](#)

Solid

► [Human Metabolome Database \(HMDB\)](#)

COLOURLESS OILY LIQUID.

► [ILO International Chemical Safety Cards \(ICSC\)](#)

practically colourless, oily liquid; bitter taste; little odour

► [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

### 3.2.2 Color/Form



Oily liquid

*O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 416*

► [Hazardous Substances Data Bank \(HSDB\)](#)

Colorless, mobile liquid

*Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1272*

► [Hazardous Substances Data Bank \(HSDB\)](#)

### 3.2.3 Odor



Fruity odor

*David RM et al; Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology. 6th ed. (1999-2015). New York, NY: John Wiley & Sons, Inc. On-line Posting Date: August 17, 2012.*

► [Hazardous Substances Data Bank \(HSDB\)](#)

### 3.2.4 Taste



Bitter taste

*O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 416*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 3.2.5 Boiling Point



294.0 °C

▶ [EPA DSSTox](#)

294 °C

Haynes, W.M. (ed.). *CRC Handbook of Chemistry and Physics. 95th Edition*. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-526

▶ [Hazardous Substances Data Bank \(HSDB\)](#); [ILO International Chemical Safety Cards \(ICSC\)](#)

### 3.2.6 Melting Point



-55 °C

Clayton, G.D., F.E. Clayton (eds.) *Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed.* New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3059

▶ [Hazardous Substances Data Bank \(HSDB\)](#); [ILO International Chemical Safety Cards \(ICSC\)](#)

<25°C

▶ [Human Metabolome Database \(HMDB\)](#)

### 3.2.7 Flash Point



155 °C (311 °F) - closed cup

Sigma-Aldrich; *Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

151 °C

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

### 3.2.8 Solubility



0.24 M

HAWLEY'S COND. CHEM. DICT. (1993)

▶ [EPA DSSTox](#)

In **water**, 6.50X10+4 mg/L at room temp

Lewis, R.J. Sr.; *Hawley's Condensed Chemical Dictionary 15th Edition*. John Wiley & Sons, Inc. New York, NY 2007., p. 1272

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

In peanut oil: 0.8%; miscible with alcohol, **ethanol**, ether

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. Cambridge, UK: Royal Society of Chemistry, 2013., p. 416

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Slightly soluble in **carbon tetrachloride**; soluble in **ethanol**, **ethyl ether**

Haynes, W.M. (ed.). *CRC Handbook of Chemistry and Physics. 95th Edition*. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-526

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

65 mg/mL

▶ [Human Metabolome Database \(HMDB\)](#)

Solubility in **water**: moderate

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

slightly soluble in **water**; miscible with alcohol and ether

▶ [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

### 3.2.9 Density



1.1369 g/cu cm at 20 °C

Haynes, W.M. (ed.). *CRC Handbook of Chemistry and Physics. 95th Edition*. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-526

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Relative density (**water** = 1): 1.1

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

1.138-1.139

▶ [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

### 3.2.10 Vapor Pressure



6.87e-04 mmHg

▶ [EPA DSSTox](#)

6.87X10<sup>-4</sup> mm Hg at 25 °C (extrapolated)

*Ohe S; Computer Aided Data Book of Vapor Pressure. Tokyo, Japan: Data Book Publ Co (1976)*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Vapor pressure, Pa at 25 °C: 0.3

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

### 3.2.11 Stability/Shelf Life



Stable under recommended storage conditions.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 3.2.12 Decomposition



When heated to decomposition it emits acrid smoke and irritating fumes.

*Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3546*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 3.2.13 Viscosity



35.2 cP at 25 °C

*O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 416*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 3.2.14 Refractive Index

[n]<sub>D</sub><sup>20</sup>: 1,439-1,441

▶ [EU Food Improvement Agents](#)

Index of refraction = 1.4455 at 20 °C/D

*Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-526*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

1.440-1.444

▶ [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

### 3.2.15 Kovats Retention Index



Standard non-polar	1655, 1627, 1655
Semi-standard non-polar	1659.4, 1656, 1659, 1630.2
Standard polar	2461

▶ [NIST Mass Spectrometry Data Center](#)

### 3.2.16 Other Experimental Properties



Pour point about 10 °C

*O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 416*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Vapor pressure = 1 mm Hg at 107.0 °C

*Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 4371*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Pour point -46 °C

*Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1272*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Henry's Law constant =  $3.8 \times 10^{-9}$  atm-cu m/mole at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of June 3, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuitedL.htm>

► [Hazardous Substances Data Bank \(HSDB\)](#)

Hydroxyl radical reaction rate constant =  $7.3 \times 10^{-12}$  cu cm/mole-sec at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of June 3, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuitedL.htm>

► [Hazardous Substances Data Bank \(HSDB\)](#)

### 3.3 SpringerMaterials Properties



[Boiling point](#)  
[Diamagnetic susceptibility](#)  
[Heat of sublimation](#)  
[Magnetic susceptibility](#)  
[Optical coefficient](#)  
[Refractive index](#)  
[Surface tension](#)  
[Vapor pressure](#)  
[Viscosity](#)

► [SpringerMaterials](#)



## 4 Spectral Information



### 4.1 1D NMR Spectra



1D NMR Spectra NMR: 150 (Sadtler Research Laboratories Spectral Collection)

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

1D NMR Spectra [1D NMR Spectrum 3321 - Triethyl citrate \(HMDB0034263\)](#)

[▶ Human Metabolome Database \(HMDB\)](#)

#### 4.1.1 1H NMR Spectra



Instrument Name	BRUKER AC-300
Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1991-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

[▶ SpectraBase](#)

Instrument Name	Varian A-60
Source of Sample	Eastman Kodak Company, Distillation Products Industries, Rochester, New York
Copyright	Copyright © 2009-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

[▶ SpectraBase](#)

#### 4.1.2 13C NMR Spectra



Showing 2 of 3 [View More](#) 

Source of Sample	Eastman Organic Chemicals, Rochester, New York
Copyright	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



▶ SpectraBase

<b>Copyright</b>	Copyright © 2016-2020 W. Robien, Inst. of Org. Chem., Univ. of Vienna. All Rights Reserved.
<b>Thumbnail</b>	

▶ SpectraBase

## 4.2 Mass Spectrometry



Showing 2 of 15 [View More](#)

<b>Source of Spectrum</b>	Chemical Concepts, A Wiley Division, Weinheim, Germany
<b>Copyright</b>	Copyright © 2002-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
<b>Thumbnail</b>	

▶ SpectraBase

<b>Instrument Name</b>	CH5
<b>Source of Spectrum</b>	Chemical Concepts, A Wiley Division, Weinheim, Germany
<b>Copyright</b>	Copyright © 2002-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
<b>Thumbnail</b>	

▶ SpectraBase

## 4.2.1 GC-MS

Showing 2 of 11 [View More](#)

GC-MS	<a href="#">GC-MS Spectrum 27482 - Triethyl citrate (HMDB0034263)</a> <a href="#">GC-MS Spectrum 28172 - Triethyl citrate (HMDB0034263)</a> <a href="#">GC-MS Spectrum 28216 - Triethyl citrate (HMDB0034263)</a> <a href="#">GC-MS Spectrum 101598 - Triethyl citrate (HMDB0034263)</a> <a href="#">GC-MS Spectrum 101599 - Triethyl citrate (HMDB0034263)</a> <a href="#">GC-MS Spectrum 101600 - Triethyl citrate (HMDB0034263)</a>
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[Human Metabolome Database \(HMDB\)](#)

MoNA ID	JP003331
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	JEOL JMS-01-SG-2
Instrument Type	EI-B
Ionization Mode	positive
Splash	splash10-0a4i-1920000000-f7c884b67f54e12797d9
Thumbnail	
Submitter	University of Tokyo Team, Faculty of Engineering, University of Tokyo

[MassBank of North America \(MoNA\)](#)

## 4.2.2 MS-MS



MS-MS	<a href="#">MS-MS Spectrum 449119 - Triethyl citrate (HMDB0034263)</a> <a href="#">MS-MS Spectrum 449120 - Triethyl citrate (HMDB0034263)</a> <a href="#">MS-MS Spectrum 449121 - Triethyl citrate (HMDB0034263)</a> <a href="#">MS-MS Spectrum 449122 - Triethyl citrate (HMDB0034263)</a> <a href="#">MS-MS Spectrum 452432 - Triethyl citrate (HMDB0034263)</a>
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[Human Metabolome Database \(HMDB\)](#)

NIST Number	1186525
Instrument Type	IT/ion trap
Collision Energy	0
Spectrum Type	MS2
Precursor Type	[M+H] <sup>+</sup>
Precursor m/z	277.1282
Total Peaks	11
m/z Top Peak	203
m/z 2nd Highest	231
m/z 3rd Highest	157
Thumbnail	

[▶ NIST Mass Spectrometry Data Center](#)

#### 4.2.3 LC-MS



Showing 2 of 5 [View More](#)

MoNA ID	<a href="#">SM878101</a>
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H] <sup>+</sup>
precursor m/z	277.1282
Instrument	Q Exactive Plus Orbitrap Thermo Scientific
Instrument Type	LC-ESI-QFT
Ionization	ESI
Ionization Mode	positive
Collision Energy	35 (nominal)
Retention Time	9.239 min
Splash	<a href="#">splash10-0a4i-0900000000-550d7ef825027f130a1e</a>
Thumbnail	
Submitter	CASMI Team, UFZ, Eawag

[▶ MassBank of North America \(MoNA\)](#)

MoNA ID	<a href="#">AU285701</a>
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H] <sup>+</sup>
precursor m/z	277.1282
Instrument	Bruker maXis Impact
Instrument Type	LC-ESI-QTOF
Ionization	ESI
Ionization Mode	positive
Collision Energy	10 eV
Retention Time	6.943 min
Splash	<a href="#">splash10-0pb9-0960000000-db7d17d9ebf75eee6344</a>
Thumbnail	

<b>Submitter</b>	Nikolaos Thomaidis, University of Athens
------------------	--

▶ [MassBank of North America \(MoNA\)](#)

#### 4.2.4 EI-MS



<b>EI-MS</b>	EI-MS Spectrum 645 - Triethyl citrate (HMDB0034263)
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▶ [Human Metabolome Database \(HMDB\)](#)

#### 4.2.5 Other MS



<b>Other MS</b>	MASS: 69960 (NIST/EPA/MSDC Mass Spectral Database, 1990 version)
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▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 4.3 IR Spectra



<b>IR Spectra</b>	IR: 6730 (Coblentz Society Spectral Collection)
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▶ [Hazardous Substances Data Bank \(HSDB\)](#)

#### 4.3.1 FTIR Spectra



Showing 2 of 6 [View More](#)

<b>Instrument Name</b>	DIGILAB FTS-40
<b>Technique</b>	NEAT
<b>Source of Sample</b>	Scientific Polymer Products, Inc.
<b>Copyright</b>	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

▶ [SpectraBase](#)

<b>Technique</b>	CAPILLARY CELL: NEAT
<b>Source of Sample</b>	Eastman Kodak Company, Distillation Products Industries, Rochester, New York
<b>Copyright</b>	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

▶ [SpectraBase](#)

#### 4.3.2 ATR-IR Spectra



Showing 2 of 4

Showing 2 of 7

[View More](#) 

<b>Instrument Name</b>	Bio-Rad FTS
<b>Technique</b>	ATR-Neat (DurasamplIR II)
<b>Source of Spectrum</b>	Forensic Spectral Research
<b>Source of Sample</b>	Scientific Polymer Products, Inc.
<b>Catalog Number</b>	P-110
<b>Lot Number</b>	080707001
<b>Copyright</b>	Copyright © 2012-2020 John Wiley & Sons, Inc. All Rights Reserved.
<b>Thumbnail</b>	

[▶ SpectraBase](#)

<b>Instrument Name</b>	Bruker Tensor 27 FT-IR
<b>Technique</b>	ATR-Neat (DuraSamplIR II)
<b>Source of Spectrum</b>	Bio-Rad Laboratories, Inc.
<b>Source of Sample</b>	Alfa Aesar, Thermo Fisher Scientific
<b>Catalog Number</b>	L12639
<b>Lot Number</b>	10129572
<b>Copyright</b>	Copyright © 2016-2020 John Wiley & Sons, Inc. All Rights Reserved.
<b>Thumbnail</b>	

[▶ SpectraBase](#)

#### 4.3.3 Near IR Spectra



<b>Technique</b>	NIR Path Length= 0.5/20 (20 = 4.5 mm) Spectrometer= BRUKER IFS 88 Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=8317,REO=2,CNM=HEI,ZFF=2
<b>Source of Spectrum</b>	Prof. Buback, University of Goettingen, Germany
<b>Copyright</b>	Copyright © 1989, 1990-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
<b>Thumbnail</b>	

[▶ SpectraBase](#)

<b>Technique</b>	NIR Path Length= 0.5/20 (20 = 4.5 mm) Spectrometer= BRUKER IFS 88 Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=8317,REO=2,CNM=HEI,ZFF=2
<b>Source of Spectrum</b>	Prof. Buback, University of Goettingen, Germany
<b>Copyright</b>	Copyright © 1989, 1990-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
<b>Thumbnail</b>	

[▶ SpectraBase](#)

#### 4.3.4 Vapor Phase IR Spectra



<b>Instrument Name</b>	DIGILAB FTS-14
<b>Technique</b>	Vapor Phase
<b>Copyright</b>	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.
<b>Thumbnail</b>	

[▶ SpectraBase](#)

#### 4.4 Raman Spectra



Showing 2 of 3 [View More](#)

<b>Raman Spectra</b>	Raman: 489 (Sadtler Research Laboratories Spectral Collection)
<a href="#">▶ Hazardous Substances Data Bank (HSDB)</a>	
<b>Instrument Name</b>	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
<b>Technique</b>	FT-Raman
<b>Source of Spectrum</b>	Bio-Rad Laboratories, Inc.
<b>Source of Sample</b>	Alfa Aesar, Thermo Fisher Scientific
<b>Catalog Number</b>	L12639
<b>Lot Number</b>	10129572
<b>Copyright</b>	Copyright © 2016-2020 John Wiley & Sons, Inc. All Rights Reserved.
<b>Thumbnail</b>	

▶ [SpectraBase](#)

## 4.5 Other Spectra



SADTLER REFERENCE NUMBER: 2402 (IR, PRISM)

Weast, R.C. (ed.). *Handbook of Chemistry and Physics*. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979, p. C-251

▶ [Hazardous Substances Data Bank \(HSDB\)](#)



## 5 Related Records



### 5.1 Related Compounds with Annotation



▶ PubChem

## 5.2 Related Compounds



Same Connectivity	2 Records
Same Parent, Connectivity	17 Records
Same Parent, Exact	16 Records
Mixtures, Components, and Neutralized Forms	48 Records
Similar Compounds	907 Records
Similar Conformers	24 Records

▶ PubChem

## 5.3 Substances



### 5.3.1 Related Substances



All	177 Records
Same	125 Records
Mixture	52 Records

▶ PubChem

### 5.3.2 Substances by Category



▶ PubChem

## 5.4 Entrez Crosslinks



PubMed	3 Records
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▶ PubChem

## 6 Chemical Vendors

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▶ PubChem

## 7 Drug and Medication Information



### 7.1 Clinical Trials



#### 7.1.1 ClinicalTrials.gov



▶ [ClinicalTrials.gov](#)

#### 7.1.2 EU Clinical Trials Register



▶ [EU Clinical Trials Register](#)

#### 7.1.3 NIPH Clinical Trials Search of Japan



▶ [NIPH Clinical Trials Search of Japan](#)

## 7.2 Therapeutic Uses



/EXPL THER/ The objective of this study was/ to evaluate the efficacy and tolerability of a novel lotion containing triethyl citrate and [ethyl linoleate](#) in the treatment of mild to moderate acne vulgaris. This was a double-blind, placebo-controlled, randomized study comparing the active lotion containing triethyl citrate and [ethyl linoleate](#) with its vehicle as a placebo control. Patients were assessed by the modified Leeds acne grading system as well as by counting inflammatory and noninflammatory lesions on the face at weeks 0, 4, 8 and 12. Sebum production was assessed by the Sebutape method at weeks 0 and 12. All adverse events were recorded. Forty patients were recruited into the study, of whom 33 completed the study. Active treatment was statistically superior to placebo in reduction of Leeds grading and total, inflammatory and noninflammatory lesion counts. The active lotion showed a rapid response with obvious reduction in lesion counts and acne grading by 4 weeks. Sebum production was significantly reduced in the actively treated group, with a mean reduction of 53% in sebum production compared with baseline. One patient developed irritation to the active lotion and withdrew from the study. The new lotion containing triethyl citrate and [ethyl linoleate](#) has been shown to be an effective treatment for mild to moderate acne, with an effect on both

inflammatory and noninflammatory acne lesions. The new lotion worked quickly and was generally well tolerated. A surprising finding was the significant impact the new lotion has on sebum production, suggesting a role in patients with seborrhea.

[PMID:17635508](#)

*Charakida A et al; Br J Dermatol 157 (3): 569-74 (2007)*

► [Hazardous Substances Data Bank \(HSDB\)](#)

MEDICATION (VET): ... Orally, in treating bloat in ruminants.

*Rossoff, I.S. Handbook of Veterinary Drugs. New York: Springer Publishing Company, 1974, p. 618*

► [Hazardous Substances Data Bank \(HSDB\)](#)

## 8 Food Additives and Ingredients

### 8.1 Food Additive Classes

Flavoring Agents

- ▶ [EU Food Improvement Agents; Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

JECFA Functional Classes

Flavoring Agents -> FLAVOURING\_AGENTFood Additives -> CARRIER\_SOLVENTFood Additives -> SEQUESTRANT

- ▶ [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

### 8.2 FEMA Flavor Profile

Fruit

- ▶ [Flavor and Extract Manufacturers Association \(FEMA\)](#)

### 8.3 FDA Substances Added to Food

Substance	<a href="#">TRIETHYL CITRATE</a>
Used for (Technical Effect)	SOLVENT OR VEHICLE
	<a href="#">175.300</a>
Document Number (21 CFR)	<a href="#">175.320</a>
	<a href="#">181.27</a>

- ▶ [FDA Center for Food Safety and Applied Nutrition \(CFSAN\)](#)

### 8.4 Organoleptic Properties

Flavors

[wine](#)  
[mild](#)  
[odorless](#)  
[fruity](#)

- ▶ [FooDB](#)

### 8.5 Evaluations of the Joint FAO/WHO Expert Committee on Food Additives - JECFA

Chemical Name	ETHYL CITRATE
Evaluation Year	1999
ADI	0-20 mg/kg bw (1984)
Comments	No safety concern at current levels of intake when used as a flavouring agent. The 1984 ADI of 0-20 mg/kg bw was maintained at the fifty-third meeting (1999).
Report	<a href="#">TRS 896-JECFA 53/67</a>

- ▶ [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

## 9 Pharmacology and Biochemistry



### 9.1 Absorption, Distribution and Excretion



In order to assess the toxicological behavior of triethyl citrate, the available experimental and predicted physico-chemical data have been evaluated. The substance is expected to be absorbed very well. The absorption of any metabolite of the substances of interest is fast and complete. Concerning the absorption after exposure via inhalation, as the chemical has a low vapor pressure, it is clear, that the substance is poorly available after inhalation. Given its lipophilicity (LogPow 1.17) - if absorbed - it is expected to be absorbed directly across the respiratory tract epithelium. The substance is expected to be also poorly absorbed following dermal exposure into the stratum corneum and to a certain extent into the epidermis, due to its molecular weight and its LogPow. In addition, the systemic toxicity via the skin is assumed to be low and this has been proven with the results of the acute dermal study with triethyl citrate, in which a LD50 of 5000 mg/kg bw has been obtained. Concerning the distribution in the body, triethyl citrate is expected to be mainly available in the circulatory system (due to its [water](#) solubility). The experimentally determined LogPow value, the [water](#) solubility and predicted behavior concerning absorption of the substance triethyl citrate do not indicate a potential for accumulation.

European Chemicals Agency (ECHA); Registered Substances, Triethyl citrate (CAS Number: 77-93-0) (EC Number: 201-070-7) (September 12, 2014). Available from, as of May 6, 2015: <http://echa.europa.eu/en/information-on-chemicals>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 9.2 Metabolism/Metabolites



Triethyl citrate is hydrolyzed in vivo to [citric acid](#) and [ethanol](#). Triethyl citrate appeared to be hydrolyzed at a slower rate with human serum compared to rat serum.

European Commission/ Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). Opinion on the Toxicological Characteristics and Risks of Certain Citrates and Adipates Used as a Substitute for Phthalates as Plasticisers in Certain Soft PVC Products. (September 1999). Available from, as of May 5, 2015: [http://ec.europa.eu/health/scientific\\_committees/environmental\\_risks/sctee/index\\_en.htm](http://ec.europa.eu/health/scientific_committees/environmental_risks/sctee/index_en.htm)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Samples of freshly collected rat or human serum were spiked with triethyl citrate and the disappearance of the triethyl citrate measured over a 4 hr period. Triethyl citrate was rapidly hydrolysed by rat serum (15 min), but hydrolysis occurred at a much slower rate in human serum and was not complete at the end of the 4 hr test period.

WHO/FAO; Expert Committee on Food Additives. Triethyl citrate (WHO Food Additives Series 19). (April 1979). Available from, as of May 5, 2015: <http://www.inchem.org/>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Rat-, mouse- and human-liver homogenates as well as serum enzymes hydrolyse triethyl citrate to 1 mol [citric acid](#) and 3 mol [ethanol](#)/mol ester.

WHO/FAO; Expert Committee on Food Additives. Triethyl citrate (WHO Food Additives Series 19). (April 1979). Available from, as of May 5, 2015: <http://www.inchem.org/>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

/Triethyl citrate/ is expected to be extensively metabolized by esterases and cytochrome P450 enzymes and break-down in the beta-oxidation or [citric acid](#) cycle or in cases subsequent glucuronidation. The substance is assumed to be excreted (if not metabolized completely in beta-oxidation and citric cycle) as metabolites (i.e. conjugates with [glucuronic acid](#)) via urine and to a lower extent via bile.

European Chemicals Agency (ECHA); Registered Substances, Triethyl citrate (CAS Number: 77-93-0) (EC Number: 201-070-7) (September 12, 2014). Available from, as of May 6, 2015: <http://echa.europa.eu/en/information-on-chemicals>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 9.3 Mechanism of Action



There was some evidence that type of effects produced may have resulted from binding of [calcium](#) by release of [citrate](#) ion with resultant hypocalcemia.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3058

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 9.4 Human Metabolite Information



#### 9.4.1 Cellular Locations



Cytoplasm  
Extracellular

▶ [Human Metabolome Database \(HMDB\)](#)

## 10 Use and Manufacturing



### 10.1 Overview



**IDENTIFICATION:** Triethyl citrate is a colorless, oily liquid. It has a fruity odor and bitter taste. Triethyl citrate is very soluble in [water](#). **USE:** Triethyl citrate is an important commercial chemical used as an industrial solvent and in paint removers. It is also used to increase the flexibility of plastics. Triethyl citrate is a food additive used in small amounts as a flavor-preserving agent and stabilizer in processed food (e.g., alcoholic and nonalcoholic beverages, packaged baked goods, frozen dairy or egg whites, gelatins and puddings, chewing gum, and candy). It is also used in various personal care products, including perfumes, body sprays, lotions, and hairsprays. **EXPOSURE:** Workers that use or produce triethyl citrate may breathe in mists or have direct skin contact. The general population may be exposed to small amounts by breathing in mists or have direct skin contact using personal care products containing triethyl citrate or by ingesting foods or medicines that contain triethyl citrate as an additive. If triethyl citrate is released to air, it will be broken down by reaction with other chemicals. It will not be broken down by light. If released to [water](#) or soil, it is not expected to bind to soil particles or suspended particles. Triethyl citrate is expected to move through soil. Triethyl citrate is not expected to move into air from wet soils or [water](#) surfaces. Triethyl citrate is expected to be broken down by microorganisms and is not expected build up in tissues of aquatic organisms. **RISK:** Neither skin irritation nor allergic reactions occurred in humans following skin exposure to a low-to-moderate dose of triethyl citrate. No other studies on human health effects following exposure to triethyl citrate were located. Allergic skin reactions and eye irritation occurred in laboratory animals exposed to moderate-to-high doses of triethyl citrate. Weakness and decreased activity followed by extreme agitation, convulsions, and death were observed in laboratory animals exposed once to a high oral dose. No effects were observed in laboratory animal fed low-to-moderate doses of triethyl citrate over time. The potential of triethyl citrate to cause infertility, abortions, or birth defects has not been examined in laboratory animals. The potential of triethyl citrate to cause cancer in laboratory animals has not been examined. The potential for triethyl citrate to cause cancer in humans has not been assessed by the U.S. EPA IRIS program, the International Agency for Research on Cancer, or the U.S. National Toxicology Program 13th Report on Carcinogens. (SRC)

FOR MORE INFORMATION: (1) National Library of Medicine Hazardous Substances Data Bank. Available from, as of Jun 5, 2015: <http://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm> (2) IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Available from, as of Jun 5, 2015: <http://monographs.iarc.fr/ENG/Classification/index.php> (3) National Library of Medicine Household Products Database. Available from, as of Jun 5, 2015: <http://hpd.nlm.nih.gov/> (4) USEPA/IRIS Integrated Risk Information System. Available from, as of Jun 5, 2015: <http://www.epa.gov/iris/> (5) Select Committee on GRAS Substances (SCOGS) Opinion: Ammonium Citrate. Available from, as of Jun 5, 2015: <http://www.fda.gov/food/ingredientspackaginglabeling/gras/scogs/ucm260861.htm>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 10.2 Use Classification



EPA Safer Chemical Functional Use Classes -> [Fragrances;Solvents](#)

▶ [EPA Safer Choice](#)

Safer Chemical Classes ->  Yellow triangle - The chemical has met Safer Choice Criteria for its functional ingredient-class, but has some hazard profile issues

▶ [EPA Safer Choice](#)

Food additives

▶ [EU Food Improvement Agents](#)

Food additives -> [Flavoring Agents](#)

▶ [EU Food Improvement Agents](#)

Flavoring Agents -> [FLAVOURING\\_AGENT](#)Food Additives -> [CARRIER\\_SOLVENT](#)Food Additives -> [SEQUESTRANT](#) -> [JECFA Functional Classes](#)

▶ [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

Flavoring Agents -> [JECFA Flavorings Index](#)

▶ [Joint FAO/WHO Expert Committee on Food Additives \(JECFA\)](#)

Cosmetics -> [Antioxidant](#); [Deodorant](#); [Plasticiser](#); [Solvent](#)

513 | [EUCOSMETICS](#) | *Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)* | [DOI:10.5281/zenodo.2624118](https://doi.org/10.5281/zenodo.2624118)

▶ [NORMAN Suspect List Exchange](#)

### 10.3 Uses



EPA CPDat Chemical and Product Categories

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, *Scientific Data*, volume 5, Article number: 180125 (2018), [DOI:10.1038/sdata.2018.125](https://doi.org/10.1038/sdata.2018.125)

▶ [EPA Chemical and Products Database \(CPDat\)](#)

Solvent and plasticizer for [nitrocellulose](#) and natural resins, softener, paint removers, agglutinant, perfume base, food additive (not over 0.25%).

Lewis, R.J. Sr.; *Hawley's Condensed Chemical Dictionary 15th Edition*. John Wiley & Sons, Inc. New York, NY 2007., p. 1272

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

#### MEDICATION (VET)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Used as a plasticizer and solvent for [cellulose nitrate](#), [cellulose acetate](#), and cellulose ethers. It can also be used as a plasticizer for PVC. It has been used as a solvent, in paint removers, in emulsifiers in food industry, and as a flavor-preserving agent.

David RM et al; *Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology*. 6th ed. (1999-2015). New York, NY: John Wiley & Sons, Inc. On-line Posting Date: August 17, 2012.

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

... optional ingredient in liquid and frozen egg white ... sometimes added as a whipping aid, as well as a gum to increase viscosity and to improve stability of the egg white foam.

Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. Volumes 1: New York, NY: John Wiley and Sons, 1991-Present., p. V8 897 (1993)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

#### Reported uses (ppm):

Table: Reported uses (ppm): (Flavor and Extract Manufacturers' Association, 1994)

Food Category	Usual	Max.
Alcoholic beverages	0.02	0.03
Baked goods	0.04	0.12
Chewing gum	0.50	0.50
Frozen dairy	0.01	0.07
Gelatins, puddings	0.01	0.02
Hard candy	0.01	0.04
Nonalcoholic beverages	0.01	0.03
Soft candy	0.03	0.08

Burdock, G.A. (ed.). *Fenaroli's Handbook of Flavor Ingredients*. 6th ed. Boca Raton, FL 2010, p. 1933

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Fixatives are used to equalize the vapor pressures, and thus the volatilities, of the raw materials in a perfume oil, as well as to increase the tenacity. ... Synthetic fixatives include substances of low volatility ([cyclopentadecanolide](#), [ambroxide](#), [benzyl salicylate](#)) and virtually odorless solvents with very low vapor pressures ([benzyl benzoate](#), [diethyl phthalate](#), triethyl citrate).

Sturm W, Peters W; *Perfumes. Ullmann's Encyclopedia of Industrial Chemistry* 7th ed. (1999-2015). NY, NY: John Wiley & Sons. Online Posting Date: June 15, 2000

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 10.3.1 Industry Uses



Odor agents  
Plasticizers  
Processing aids, not otherwise listed  
Solvents (which become part of product formulation or mixture)

<https://www.epa.gov/chemical-data-reporting>

▶ [EPA Chemicals under the TSCA](#)

### 10.3.2 Consumer Uses



Air care products  
Cleaning and furnishing care products  
Laundry and dishwashing products  
Paper products  
Personal care products  
Plastic and rubber products not covered elsewhere  
Toys, playground, and sporting equipment

<https://www.epa.gov/chemical-data-reporting>

▶ [EPA Chemicals under the TSCA](#)

## 10.4 Methods of Manufacturing



By esterification of [ethyl alcohol](#) with [citric acid](#).

Burdock, G.A. (ed.). *Fenaroli's Handbook of Flavor Ingredients*. 6th ed. Boca Raton, FL 2010, p. 1933

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 10.5 Formulations/Preparations



Grades: Technical; refined; Food Chemical Codex

Lewis, R.J. Sr.; *Hawley's Condensed Chemical Dictionary 15th Edition*. John Wiley & Sons, Inc. New York, NY 2007., p. 1272

▶ [Hazardous Substances Data Bank \(HSDB\)](#)





## 10.6 U.S. Production

### Aggregated Product Volume (EPA CDR 2016)

1,000,000 - 10,000,000 lb

<https://www.epa.gov/chemical-data-reporting>

▶ [EPA Chemicals under the TSCA](#)

(1975) PROBABLY GREATER THAN 4.54X10+5 GRAMS

*SRI*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Production volume for non-confidential chemicals reported under the 2006 Inventory Update Rule. Chemical: **1,2,3-Propanetricarboxylic acid, 2-hydroxy-, 1,2,3-triethyl ester**. Aggregated National Production Volume: 1 to < 10 million pounds.

*US EPA; Non-Confidential 2006 Inventory Update Reporting. National Chemical Information. 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, 1,2,3-triethyl ester (77-93-0). Available from, as of April 23, 2015: <http://cfpub.epa.gov/iursearch/index.cfm>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Non-confidential 2012 Chemical Data Reporting (CDR) information on the production and use of chemicals manufactured or imported into the United States. Chemical: **1,2,3-Propanetricarboxylic acid, 2-hydroxy-, 1,2,3-triethyl ester**. National Production Volume: 1,000,000 - 10,000,000 lb/yr.

*USEPA/Pollution Prevention and Toxics; 2012 Chemical Data Reporting Database. 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, 1,2,3-triethyl ester (77-93-0). Available from, as of April 24, 2015: [http://java.epa.gov/oppt\\_chemical\\_search/](http://java.epa.gov/oppt_chemical_search/)*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 10.7 General Manufacturing Information



### Industry Processing Sectors

All other chemical product and preparation manufacturing  
Food, beverage, and tobacco product manufacturing  
Fragrances  
Pharmaceutical and medicine manufacturing  
Plastics product manufacturing  
Soap, cleaning compound, and toilet preparation manufacturing

▶ [EPA Chemicals under the TSCA](#)

### EPA TSCA Commercial Activity Status

**1,2,3-Propanetricarboxylic acid, 2-hydroxy-, 1,2,3-triethyl ester**: ACTIVE

<https://www.epa.gov/tsc-a-inventory>

▶ [EPA Chemicals under the TSCA](#)

## 11 Identification



### 11.1 Analytic Laboratory Methods



Method: USGS-NWQL O-1433-01; Procedure: gas chromatography/mass spectrometry; Analyte: triethyl citrate; Matrix: filtered wastewater and natural-[water](#) samples; Detection Limit: 0.09 ug/L.

*National Environmental Methods Index; Analytical, Test and Sampling Methods. Triethyl Citrate (77-93-0). Available from, as of April 29, 2015: <http://www.nemi.gov>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Method: USGS-NWQL O-4433-06; Procedure: continuous liquid-liquid extractor with gas chromatography with mass spectrometry detection; Analyte: triethyl citrate; Matrix: whole wastewater and environmental [water](#) samples; Detection Limit: 0.07 ug/L.

*National Environmental Methods Index; Analytical, Test and Sampling Methods. Triethyl Citrate (77-93-0). Available from, as of April 29, 2015: <http://www.nemi.gov>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 12 Safety and Hazards



### 12.1 Hazards Identification



#### 12.1.1 GHS Classification



Showing 1 of 2 [View More](#)

**GHS Hazard Statements** Not Classified  
Reported as not meeting GHS hazard criteria by 1827 of 1896 companies (only ~ 3.6% companies provided GHS information). For more detailed information, please visit [ECHA C&L website](#).

▶ [European Chemicals Agency \(ECHA\)](#)

#### 12.1.2 EPA Safer Chemical



Chemical: Triethyl citrate

Yellow triangle - The chemical has met Safer Choice Criteria for its functional ingredient-class, but has some hazard profile issues. Specifically, a chemical with this code is not associated with a low level of hazard concern for all human health and environmental endpoints. (See [Safer Choice Criteria](#)). While it is a best-in-class chemical and among the safest available for a particular function, the function fulfilled by the chemical should be considered an area for safer chemistry innovation.

▶ [EPA Safer Choice](#)

#### 12.1.3 Fire Hazards



Combustible.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

#### 12.1.4 Fire Potential



Combustible liquid when exposed to heat or flame.

*Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3546*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 12.2 First Aid Measures



### 12.2.1 Inhalation First Aid



Fresh air, rest.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

### 12.2.2 Skin First Aid



Remove contaminated clothes. Rinse skin with plenty of **water** or shower.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

### 12.2.3 Eye First Aid



First rinse with plenty of **water** for several minutes (remove contact lenses if easily possible), then refer for medical attention.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

### 12.2.4 Ingestion First Aid



Rinse mouth. Give one or two glasses of **water** to drink.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

## 12.3 Fire Fighting



Use powder, **carbon dioxide**.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

### 12.3.1 Fire Fighting Procedures



Suitable extinguishing media: Use **water** spray, alcohol-resistant foam, dry chemical or **carbon dioxide**.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Advice for firefighters: Wear self contained breathing apparatus for fire fighting if necessary.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Use dry chemical, [carbon dioxide](#).

*Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3546*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 12.4 Accidental Release Measures

### 12.4.1 Spillage Disposal

Collect leaking and spilled liquid in sealable containers as far as possible. Wash away remainder with plenty of [water](#).

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

### 12.4.2 Cleanup Methods

Accidental release measures: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation.; Environmental precautions: Do not let product enter drains.; Methods and materials for containment and cleaning up: Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 12.4.3 Disposal Methods

SRP: Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in air, soil or [water](#); effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contaminated packaging: Dispose of as unused product.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 12.4.4 Preventive Measures

Precautions for safe handling: Avoid contact with skin and eyes. Avoid inhalation of vapor or mist. Normal measures for preventive fire protection.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Appropriate engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 12.5 Handling and Storage

### 12.5.1 Safe Storage

Well closed.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

### 12.5.2 Storage Conditions

Keep container tightly closed in a dry and well-ventilated place.

*Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 12.6 Exposure Control and Personal Protection

### 12.6.1 Inhalation Risk

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20 °C.

▶ ILO International Chemical Safety Cards (ICSC)

## 12.6.2 Effects of Short Term Exposure



The substance is irritating to the eyes and respiratory tract.

▶ ILO International Chemical Safety Cards (ICSC)

## 12.6.3 Allowable Tolerances



Unless specifically excluded, residues resulting from the use of the following substance as either an inert or an active ingredient in a pesticide chemical formulation, including antimicrobial pesticide chemicals, is exempted from the requirement of a tolerance under FFDC section 408, if such use is in accordance with good agricultural or manufacturing practices. Citric acid, triethyl ester is included on this list.

40 CFR 180.950 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of April 20, 2015: <http://www.ecfr.gov>

▶ Hazardous Substances Data Bank (HSDB)

## 12.6.4 Personal Protective Equipment (PPE)



**Eye/face protection:** Face shield and safety glasses. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>

▶ Hazardous Substances Data Bank (HSDB)

**Skin protection:** Handle with gloves.

Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>

▶ Hazardous Substances Data Bank (HSDB)

**Body Protection:** Complete suit protecting against chemicals. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>

▶ Hazardous Substances Data Bank (HSDB)

**Respiratory protection:** Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>

▶ Hazardous Substances Data Bank (HSDB)

## 12.6.5 Fire Prevention



NO open flames.

▶ ILO International Chemical Safety Cards (ICSC)

## 12.6.6 Inhalation Prevention



Use ventilation, local exhaust or breathing protection.

▶ ILO International Chemical Safety Cards (ICSC)

## 12.6.7 Skin Prevention



Protective gloves.

▶ ILO International Chemical Safety Cards (ICSC)

## 12.6.8 Eye Prevention



Wear safety spectacles or eye protection in combination with breathing protection.

▶ ILO International Chemical Safety Cards (ICSC)

## 12.6.9 Ingestion Prevention



Do not eat, drink, or smoke during work.

▶ ILO International Chemical Safety Cards (ICSC)

## 12.7 Stability and Reactivity



### 12.7.1 Hazardous Reactivities and Incompatibilities



Incompatible materials: Strong oxidizing agents

Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 12.8 Regulatory Information



### 12.8.1 FIFRA Requirements



Unless specifically excluded, residues resulting from the use of the following substance as either an inert or an active ingredient in a pesticide chemical formulation, including antimicrobial pesticide chemicals, is exempted from the requirement of a tolerance under FFDCFA section 408, if such use is in accordance with good agricultural or manufacturing practices. Citric acid, triethyl ester is included on this list.

40 CFR 180.950 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of April 20, 2015: <http://www.ecfr.gov>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 12.8.2 FDA Requirements



An ingredient whose use in food or food packaging is subject to a prior sanction or approval within the meaning of section 201(s)(4) of the Act is exempt from classification as a food additive. ... Substances classified as plasticizers, when migrating from food-packaging material shall include ... triethyl citrate.

21 CFR 181.27 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of April 20, 2015: <http://www.ecfr.gov>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Substance added directly to human food affirmed as generally recognized as safe (GRAS).

21 CFR 184.1911 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of April 20, 2015: <http://www.ecfr.gov>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 12.9 Other Safety Information



### 12.9.1 Toxic Combustion Products



Special hazards arising from the substance or mixture: Carbon oxides

Sigma-Aldrich; Material Safety Data Sheet for Triethyl citrate. Product Number: W308307, Version 3.9 (Revision Date 07/09/2014). Available from, as of April 29, 2015: <http://www.sigmaaldrich.com/safety-center.html>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 13 Toxicity



### 13.1 Toxicological Information



#### 13.1.1 NIOSH Toxicity Data



▶ [The National Institute for Occupational Safety and Health \(NIOSH\)](#)

#### 13.1.2 Exposure Routes



The substance can be absorbed into the body by inhalation of its aerosol and by ingestion.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

#### 13.1.3 Inhalation Symptoms



Cough.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

#### 13.1.4 Eye Symptoms



Redness.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

#### 13.1.5 Ingestion Symptoms



Vomiting.

▶ [ILO International Chemical Safety Cards \(ICSC\)](#)

#### 13.1.6 Acute Effects



▶ [ChemIDplus](#)

#### 13.1.7 Toxicity Summary



IDENTIFICATION AND USE: Triethyl citrate is a colorless, oily liquid with bitter taste. It is used as solvent and plasticizer for [nitrocellulose](#) and natural resins, softener, paint removers, agglutinant, perfume base, food additive (not over 0.25%) as an emulsifier and as a flavor-preserving agent. HUMAN EXPOSURE AND TOXICITY: Triethyl citrate 20% in petrolatum was not a primary irritant or sensitizer in human studies. ANIMAL STUDIES: Triethyl citrate, applied undiluted during epidermal induction, was a strong sensitizer in a guinea pig maximization test. Triethyl citrate 33.3% produced irritation in rabbit eyes. Intravenous administration of a 100 mg/kg bw dose of triethyl citrate to rabbits produced a marked increase in motor activity and respiration. A group of 20 mice given

intraperitoneal doses of 350 mg/kg bw of triethyl citrate daily for 14 days had a slightly lower mean growth rate than control animals. No differences were seen in the two groups in erythrocyte and leucocyte blood cell count, clotting time and hemoglobin levels. Examination of the liver, lung and kidney tissues of two animals at necropsy revealed no pathological cellular changes. At doses ranging from 0.5 to 10 mg/kg b.w. triethyl citrate was nonteratogenic in the chicken embryo. Ames test using triethyl citrate (0.4%-1.6%) on *Salmonella typhimurium* TA1535, TA1537, TA1538 was negative with and without metabolic activation.

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.1.8 Antidote and Emergency Treatment



Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Esters and related compounds/

*Currence, P.L. Clements, B., Bronstein, A.C. (Eds.); Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 253*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... Monitor for shock and treat if necessary ... For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport ... Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal ... /Esters and related compounds/

*Currence, P.L. Clements, B., Bronstein, A.C. (Eds.); Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 253*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques with a bag-valve-mask device may be beneficial. Consider drug therapy for pulmonary edema ... Monitor cardiac rhythm and treat arrhythmias as necessary ... Start an IV with D5W TKO /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Consider vasopressors if patient is hypotensive with a normal fluid volume. Watch for signs of fluid overload ... Use proparacaine hydrochloride to assist eye irrigation ... /Esters and related compounds/

*Currence, P.L. Clements, B., Bronstein, A.C. (Eds.); Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 254*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.1.9 Human Toxicity Excerpts



/HUMAN EXPOSURE STUDIES/ Triethyl citrate 20% in pet (petrolatum) was not a primary irritant or sensitizer in human studies.

*Cosmetic Ingredient Review; Safety Assessment of Citric Acid, Inorganic Citrate Salts, and Alkyl Esters as Used in Cosmetics. Int J Toxicol 33 (2 suppl): 165-46S. (Epub ahead of print) (2014) <http://www.cir-safety.org/ingredients>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

/OTHER TOXICITY INFORMATION/ Due to its sensitizing potential ... triethyl citrate /is not considered/ to be a suitable substitute for phthalates as plasticizers in children's toys.

*European Commission/ Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). Opinion on the Toxicological Characteristics and Risks of Certain Citrates and Adipates Used as a Substitute for Phthalates as Plasticisers in Certain Soft PVC Products. p.18 (September 1999). Available from, as of May 5, 2015: [http://ec.europa.eu/health/scientific\\_committees/environmental\\_risks/sctee/index\\_en.htm](http://ec.europa.eu/health/scientific_committees/environmental_risks/sctee/index_en.htm)*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.1.10 Non-Human Toxicity Excerpts



/LABORATORY ANIMALS: Acute Exposure/ The corneal reflex in rabbit eyes was temporarily eliminated upon instillation of 3 drops of a 5% suspension of triethyl ... citrate in 3% acacia ... The anesthetic effect was confirmed by the intradermal administration of 0.1 mL of a 2% solution of triethyl ... citrate into an area of the shaved back of guinea pigs. Triethyl citrate resulted in insensitivity to pricking of the area lasting 12 to 20 minutes ...

*Cosmetic Ingredient Review; Safety Assessment of Citric Acid, Inorganic Citrate Salts, and Alkyl Esters as Used in Cosmetics. Int J Toxicol 33 (2 suppl): 165-46S. (Epub ahead of print) (2014) <http://www.cir-safety.org/ingredients>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

/LABORATORY ANIMALS: Acute Exposure/ Symptoms produced by single oral doses of ... triethyl /citrate/ are similar in both rats and cats include signs of weakness, depression and finally hyperirritability with convulsions and respiratory failure. Onset of symptoms was quite rapid ... in some cases symptoms continued for 2 days.

*Patty, F. (ed.). Industrial Hygiene and Toxicology: Volume II: Toxicology. 2nd ed. New York: Interscience Publishers, 1963., p. 1892*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

/LABORATORY ANIMALS: Acute Exposure/ Intravenous administration of a 100 mg/kg bw dose of triethyl citrate to rabbits produced a marked increase in motor activity and respiration.

*WHO/FAO; Expert Committee on Food Additives. Triethyl citrate (WHO Food Additives Series 14). (April 1979). Available from, as of May 5, 2015: <http://www.inchem.org/>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

/LABORATORY ANIMALS: Acute Exposure/ Triethyl citrate, applied undiluted during epidermal induction, was a strong sensitizer in a guinea pig maximization test.

*Cosmetic Ingredient Review; Safety Assessment of Citric Acid, Inorganic Citrate Salts, and Alkyl Esters as Used in Cosmetics. Int J Toxicol 33 (2 suppl): 165-46S. (Epub ahead of print) (2014) <http://www.cir-safety.org/ingredients>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

For more Non-Human Toxicity Excerpts (Complete) data for TRIETHYL CITRATE (20 total), please visit the [HSDB record page](#).

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.1.11 Non-Human Toxicity Values



Showing 5 of 11 [View More](#)

LD50 Guinea pig dermal >10 mL/kg

*Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3058*



[▶ Hazardous Substances Data Bank \(HSDB\)](#)

#### LD50 Mouse ip 1750 mg/kg

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3546

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

#### LD50 Rabbit dermal > 5 g/kg

*Cosmetic Ingredient Review; Safety Assessment of Citric Acid, Inorganic Citrate Salts, and Alkyl Esters as Used in Cosmetics*. *Int J Toxicol* 33 (2 suppl): 165-465. (Epub ahead of print) (2014) <http://www.cir-safety.org/ingredients>

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

#### LD50 Rat inhalation 3500 ppm

Clayton, G.D., F.E. Clayton (eds.) *Patty's Industrial Hygiene and Toxicology*. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3058

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

#### LD50 Rat oral 5900 mg/kg

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3546

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

### 13.1.12 Ongoing Test Status



EPA has released the first beta version (version 0.5) of the Interactive Chemical Safety for Sustainability (iCSS) Dashboard. The beta version of the iCSS Dashboard provides an interactive tool to explore rapid, automated (or in vitro high-throughput) chemical screening data generated by the Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st century (Tox21) collaboration. /The title compound was tested by ToxCast and/or Tox21 assays; Click on the "Chemical Explorer" button on the tool bar to see the data./[USEPA; ICSS Dashboard Application; Available from, as of April 22, 2015: <http://actor.epa.gov/dashboard/>]

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

## 13.2 Ecological Information



### 13.2.1 Environmental Fate/Exposure Summary



Triethyl citrate's production and use in cosmetics and personal care products and as a specialty solvent, plasticizer and food additive may result in its release to the environment through various waste streams. If released to air, a vapor pressure of 6.87X10<sup>-4</sup> mm Hg at 25 °C indicates triethyl citrate will exist solely as a vapor in the atmosphere. Vapor-phase triethyl citrate will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 4 days. Triethyl citrate does not contain chromophores that absorb at wavelengths >290 nm and, therefore, is not expected to be susceptible to direct photolysis by sunlight. If released to soil, triethyl citrate is expected to have very high mobility based upon an estimated Koc of 20. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 3.8X10<sup>-9</sup> atm-cu m/mole. Triethyl citrate is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Biodegradation data in soil or water were not available. Based on a structurally similar compound, **acetyl tributyl citrate**, which achieved 82% of the Theoretical BOD in 4 weeks utilizing the Japanese MITI test, biodegradation may be an important environmental fate process for triethyl citrate in soil and water. If released into water, triethyl citrate is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. A base-catalyzed second-order hydrolysis rate constant of 1.3X10<sup>-2</sup> L/mole-sec was estimated using a structure estimation method; this corresponds to half-lives of 16 and 2 years at pH values of 7 and 8, respectively. Occupational exposure to triethyl citrate may occur through dermal contact with this compound at workplaces where triethyl citrate is produced or used. Use data indicate that the general population may be exposed to triethyl citrate via ingestion of food and dermal contact with consumer products containing triethyl citrate. (SRC)

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.2 Artificial Pollution Sources



Triethyl citrate's production and use in cosmetics and personal care products(1,4), as a specialty solvent, plasticizer(2) and food additive(2,3) may result in its release to the environment through various waste streams(SRC).

(1) *CosmeticsINFO.org*. Washington, DC. Available from, as of June 3, 2015: <http://www.cosmeticsinfo.org> (2) David RM et al; *Esters of Mono-, Di-, and Tricarboxylic Acids*. *Patty's Toxicology*. 6th ed. (1999-2015). New York, NY: John Wiley & Sons, Inc. On-line Posting Date: 17 Aug 2012. (3) Somogyi LP; *Food Additives*. *Kirk-Othmer Encyclopedia of Chemical Technology*. (1999-2015). New York, NY: John Wiley & Sons. Online Posting Date: 18 Jun 2004. (4) Clausen T et al; *Hair Preparations*. *Ullmann's Encyclopedia of Industrial Chemistry*. 7th ed. (1999-2015). New York, NY: John Wiley & Sons. Online Posting Date: July 15, 2006.

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.3 Environmental Fate



TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 20(SRC), determined from a structure estimation method(2), indicates that triethyl citrate is expected to have very high mobility in soil(SRC). Volatilization of triethyl citrate from moist soil surfaces is not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 3.8X10<sup>-9</sup> atm-cu m/mole(SRC) based upon its vapor pressure, 6.87X10<sup>-4</sup> mm Hg(3), and water solubility, 6.5X10<sup>+4</sup> mg/L(5). Triethyl citrate is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(4). Biodegradation data in soil were not available(SRC, 2015). Based on data for **acetyl tributyl citrate**, a structural analog, triethyl citrate may be expected to biodegrade rapidly(SRC). Utilizing the Japanese MITI test **acetyl tributyl citrate**, present at 100 mg/L, reached 82% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L(5) suggesting that biodegradation of triethyl citrate may be an important environmental fate process in soil(SRC).

(1) Swann RL et al; *Res Rev* 85: 17-28 (1983) (2) US EPA; *Estimation Program Interface (EPI) Suite*. Ver. 4.1. Nov. 2012. Available from, as of June 4, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.htm> (3) Ohe S; *Computer Aided Data Book of Vapor Pressure*. Tokyo, Japan: Data Book Publ Co (1976) (4) Lewis RJ, Sr; *Hawley's Condensed Chemical Dictionary* 15th ed. New York, NY: John Wiley & Sons, Inc. P. 1272 (2007) (5) NITE; *Chemical Risk Information Platform (CHRIP)*. *Biodegradation and Bioconcentration*. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of June 2, 2015: <http://www.safe.nite.go.jp/english/db.html>

[▶ Hazardous Substances Data Bank \(HSDB\)](#)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 20(SRC), determined from a structure estimation method(2), indicates that triethyl citrate is not expected to adsorb to suspended solids and sediment(SRC). Volatilization from water surfaces is not expected(3) based upon an estimated Henry's Law constant of 3.8X10<sup>-9</sup> atm-cu m/mole(SRC) derived from its vapor pressure, 6.87X10<sup>-4</sup> mm Hg(4), and water solubility, 6.5X10<sup>+4</sup> mg/L(5). According to a classification scheme(6), an estimated BCF of 3(SRC), from an estimated log Kow of 0.33(2) and a regression-derived equation(2), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Biodegradation data in water were not available(SRC, 2015). Based on data for **acetyl tributyl citrate**, a structural analog, triethyl citrate may be expected to biodegrade rapidly(SRC). Utilizing the Japanese MITI test **acetyl tributyl citrate**, present at 100 mg/L, reached 82% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L(7) suggesting that biodegradation of triethyl citrate may be an important environmental fate process in water(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of June 4, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (4) Ohe S; Computer Aided Data Book of Vapor Pressure. Tokyo, Japan: Data Book Publ Co (1976) (5) Lewis RJ, Sr; Hawley's Condensed Chemical Dictionary 15th ed. New York, NY: John Wiley & Sons, Inc. P. 1272 (2007) (6) Franke C et al; Chemosphere 29: 1501-14 (1994) (7) NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of June 2, 2015: <http://www.safe.nite.go.jp/english/db.html>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

**ATMOSPHERIC FATE:** According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), triethyl citrate, which has a vapor pressure of 6.87X10<sup>-4</sup> mm Hg at 25 °C(2), is expected to exist solely as a vapor in the ambient atmosphere. Vapor-phase triethyl citrate is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be 4 days(SRC), calculated from its rate constant of 7.3X10<sup>-12</sup> cu cm/molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(3). Triethyl citrate does not contain chromophores that absorb at wavelengths >290 nm(4) and, therefore, is not expected to be susceptible to direct photolysis by sunlight(SRC).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Ohe S; Computer Aided Data Book of Vapor Pressure. Tokyo, Japan: Data Book Publ Co (1976) (3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12 (1990)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.4 Environmental Biodegradation



**AEROBIC:** Biodegradation data in soil and water were not available for triethyl citrate(SRC, 2015). Based on data for [acetyl tributyl citrate](#) (CAS 77-90-7), a structural analog, triethyl citrate is expected to biodegrade rapidly(SRC). Utilizing the Japanese MITI test [acetyl tributyl citrate](#), present at 100 mg/L, reached 82% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L(1).

(1) NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of June 2, 2015: <http://www.safe.nite.go.jp/english/db.html>

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.5 Environmental Abiotic Degradation



The rate constant for the vapor-phase reaction of triethyl citrate with photochemically-produced hydroxyl radicals has been estimated as 7.3X10<sup>-12</sup> cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 4 days at an atmospheric concentration of 5X10<sup>+5</sup> hydroxyl radicals per cu cm(1). A base-catalyzed second-order hydrolysis rate constant of 1.3X10<sup>-2</sup> L/mole-sec(SRC) was estimated using a structure estimation method(2); this corresponds to half-lives of 16 and 2 years at pH values of 7 and 8, respectively(2). Triethyl citrate does not contain chromophores that absorb at wavelengths >290 nm(3) and, therefore, is not expected to be susceptible to direct photolysis by sunlight(SRC).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of June 3, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5, 8-12 (1990)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.6 Environmental Bioconcentration



An estimated BCF of 3 was calculated in fish for triethyl citrate(SRC), using an estimated log Kow of 0.33(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low.

(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of June 4, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (2) Franke C et al; Chemosphere 29: 1501-14 (1994)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.7 Soil Adsorption/Mobility



Using a structure estimation method based on molecular connectivity indices(1), the Koc of triethyl citrate can be estimated to be 20(SRC). According to a classification scheme(2), this estimated Koc value suggests that triethyl citrate is expected to have very high mobility in soil.

(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of June 4, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (2) Swann RL et al; Res Rev 85: 17-28 (1983)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.8 Volatilization from Water/Soil



The Henry's Law constant for triethyl citrate is estimated as 3.8X10<sup>-9</sup> atm-cu m/mole(SRC) derived from its vapor pressure, 6.87X10<sup>-4</sup> mm Hg(1), and water solubility, 6.5X10<sup>+4</sup> mg/L(2). This Henry's Law constant indicates that triethyl citrate is expected to be essentially nonvolatile from water surfaces(3). Triethyl citrate's estimated Henry's Law constant indicates that volatilization from moist soil surfaces is not expected to occur(SRC). Triethyl citrate is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(1).

(1) Ohe S; Computer Aided Data Book of Vapor Pressure. Tokyo, Japan: Data Book Publ Co (1976) (2) Lewis RJ, Sr; Hawley's Condensed Chemical Dictionary 15th ed. New York, NY: John Wiley & Sons, Inc. P. 1272 (2007) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.9 Environmental Water Concentrations



**DRINKING WATER:** Triethyl citrate was detected in 12 stream and raw water samples taken at various locations in a drinking water treatment facility during November and December 2001. A detection frequency of 50% and a maximum concentration in finished water of 0.062 ug/L was reported (method reporting level = 0.5 ug/L). The facility is located in a heavily populated, highly urbanized drainage basin(1).

(1) Stackelberg PE et al; Sci Total Environ 329: 99-113 (2004)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

**SURFACE WATER:** Triethyl citrate was detected in water samples collected from Assunpink Creek in Trenton, NJ, 100 yards downstream from where a major WWTP discharges tertiary treated effluent and 2 miles further down at concentrations ranging from 78 to <500 ng/L and 66 to <500 ng/L, respectively(1). Assunpink creek is a tributary to the Delaware River which is used for a source of drinking water serving the city of Philadelphia and surrounding metropolitan areas(1). Triethyl citrate was detected at a median concentration of <0.5 ug/L and a maximum of 0.074 ug/L with a detection frequency of 11% in surface water samples from upstream of 10 waste water treatment plants located around the country (Arizona, Colorado, Georgia, Iowa, Kansas, Minnesota, Nevada, New Jersey, New York, South Dakota)(2). Triethyl citrate was detected in water samples collected from streams in north central and north western Arkansas in March, April and August 2004. Reported concentrations were below the reporting limit of 0.5 ug/L and estimated between 0.009 and 0.063 ug/L with a median value of 0.018 ug/L and a detection frequency of 43%(3). Triethyl citrate was detected in samples from 30 rivers taken in low flow conditions in Iowa in 2001 at maximum concentration of 0.17 ug/L with a detection frequency of 16.7%; it was not detected in medium and high flow condition samples(4).

(1) Alvarez DA; et al; Chemosphere 61: 610-22 (2005) (2) Glassmeyer ST et al; Environ Sci Technol 39: 5157-69 (2005) (3) Haggard BE; J Environ Qual 35: 1078-87 (2006) (4) Kolpin DW et al; Sci Total Environ 348: 119-30 (2004)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.10 Effluent Concentrations



Triethyl citrate was identified in the column inflow at the beginning of an experiment on May 29, 2001 below the reporting limit of 0.500 ug/L but reported as 0.200 ug/L and at the end of the experiment Jun 20, 2001 concentrations were reported as below the reporting limit of 0.500 ug/L. The concentration in the column drainage at the end of the experiment Jun 20, 2001 was also below the reporting limit of 0.500 ug/L(1). Treated effluent was applied to the top of a 2.4 meter soil column over 23 days. The soil was packed with a Mohall-Laveen sandy loam from an area northwest of Phoenix, AZ with no known history of cultivation or irrigation. Secondary treated effluent from a 17.5 million gallon/day municipal waste [water](#) treatment plant serving 120,000-150,000 residents near Phoenix, AZ was employed(1). Triethyl citrate was identified in effluent samples that receive domestic waste waters of 50,000 inhabitants of Southern Finland(2). Triethyl citrate was detected (reporting limit 0.5 ug/L) at a median concentration of 0.270 ug/L and a maximum of 0.52 ug/L with a detection frequency of 100% in [water](#) samples from 10 waste [water](#) treatment plants located around the country (Arizona, Colorado, Georgia, Iowa, Kansas, Minnesota, Nevada, New Jersey, New York, South Dakota)(3). Triethyl citrate was detected (reporting limit 0.5 ug/L) at a median concentration of 0.105 ug/L and a maximum of 0.400 ug/L with a detection frequency of 100% in [water](#) samples downstream (96 to 14,484 meters) and at a median concentration of 0.082 ug/L and a maximum of 0.26 ug/L with a detection frequency of 70% in [water](#) samples downstream (805 to 96,561 meters) from 10 waste [water](#) treatment plants located around the country (Arizona, Colorado, Georgia, Iowa, Kansas, Minnesota, Nevada, New Jersey, New York, South Dakota)(3).

(1) Cordy GE et al; *Ground Water Monit Remed* 24: 58-69 (2004) (2) Jernberg J; *Sci Total Environ* 450-451: 1-6 (2013) (3) Glassmeyer ST et al; *Environ Sci Technol* 39: 5157-69 (2005)

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

### 13.2.11 Probable Routes of Human Exposure



According to the 2012 [TSCA](#) Inventory Update Reporting data, 9 reporting facilities estimate the number of persons reasonably likely to be exposed during the manufacturing, processing, or use of triethyl citrate in the United States may be as low as <10 workers and as high as 99 workers per plant; the data may be greatly underestimated due to confidential business information (CBI) or unknown values(1).

(1) US EPA; *Chemical Data Reporting (CDR). Non-confidential 2012 Chemical Data Reporting information on chemical production and use in the United States. Available from, as of June 3, 2015: [http://www.epa.gov/cdr/pubs/guidance/cdr\\_factsheets.html](http://www.epa.gov/cdr/pubs/guidance/cdr_factsheets.html)*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

NIOSH (NOES Survey 1981-1983) has statistically estimated that 11,496 workers (3,993 of these are female) were potentially exposed to triethyl citrate in the US(1). Occupational exposure to triethyl citrate may occur through dermal contact with this compound at workplaces where triethyl citrate is produced or used. Use data indicate that the general population may be exposed to triethyl citrate via ingestion of food and dermal contact with consumer products containing triethyl citrate(SRC).

(1) NIOSH; *NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Citric acid, triethyl ester. Available from, as of June 3, 2015: <http://www.cdc.gov/noes/>*

▶ [Hazardous Substances Data Bank \(HSDB\)](#)

## 14 Literature



### 14.1 NLM Curated PubMed Citations



► PubChem

### 14.2 Springer Nature References



► Springer Nature

### 14.3 Depositor Provided PubMed Citations



► PubChem

### 14.4 Metabolite References



▶ [Human Metabolome Database \(HMDB\)](#)

## 14.5 Chemical Co-Occurrences in Literature

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▶ [PubChem](#)

## 14.6 Chemical-Gene Co-Occurrences in Literature

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▶ [PubChem](#)

## 14.7 Chemical-Disease Co-Occurrences in Literature

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▶ [PubChem](#)

## 15 Patents



### 15.1 Depositor-Supplied Patent Identifiers



▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

### 15.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=DOOTYTYQINUNNV-UHFFFAOYSA-N>

▶ PATENTSCOPE (WIPO)

## 16 Biological Test Results

---



### 16.1 BioAssay Results

---



► [PubChem](#)

## 17 Classification



### 17.1 Ontologies



#### 17.1.1 MeSH Tree



► Medical Subject Headings (MeSH)

#### 17.1.2 KEGG: Additive



► KEGG

#### 17.1.3 EPA Safer Choice



► EPA Safer Choice

#### 17.1.4 ChemIDplus





▶ ChemIDplus

#### 17.1.5 UN GHS Classification

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▶ UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

#### 17.1.6 EPA CPDat Classification

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▶ EPA Chemical and Products Database (CPDat)

#### 17.1.7 NORMAN Suspect List Exchange Classification

---



▶ NORMAN Suspect List Exchange

#### 17.1.8 EPA DSSTox Classification

---



▶ EPA DSSTox

## 18 Information Sources



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- ChemIDplus**  
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*Triethyl citrate [NF]*  
<https://chem.nlm.nih.gov/chemidplus/sid/0000077930>  
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*Triethyl citrate*  
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*Triethyl citrate*  
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<https://clinicaltrials.gov/>
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*triethyl citrate*  
<https://comptox.epa.gov/dashboard/DTXSID0040701#exposure>  
*EPA CPDat Classification*

<https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat>

## 12. EU Food Improvement Agents

TRIETHYL CITRATE

<https://eur-lex.europa.eu/legal-content/EN/ALL/?uri=CELEX%3A32012R0231>

Triethyl citrate

<https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32012R0872>

## 13. Joint FAO/WHO Expert Committee on Food Additives (JECFA)

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Triethyl citrate

<http://www.fao.org/food/food-safety-quality/scientific-advice/jecfa/jecfa-flav/details/en/c/167/>

ETHYL CITRATE

<https://apps.who.int/food-additives-contaminants-jecfa-database/chemical.aspx?chemID=3197>

## 14. EPA Safer Choice

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<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

Triethyl citrate

<https://www.epa.gov/saferchoice/safer-ingredients>

EPA Safer Chemical Ingredients Classification

<https://www.epa.gov/saferchoice>

## 15. NORMAN Suspect List Exchange

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NORMAN Suspect List Exchange Classification

<https://www.norman-network.com/nds/SLE/>

## 16. EU Clinical Trials Register

<https://www.clinicaltrialsregister.eu/>

## 17. FDA Center for Food Safety and Applied Nutrition (CFSAN)

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TRIETHYL CITRATE

<https://www.cfsanappsexternal.fda.gov/scripts/fdcc/index.cfm?set=FoodSubstances&id=TRIETHYLCITRATE>

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8Z96QXD6UM

<https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/>

## 19. Flavor and Extract Manufacturers Association (FEMA)

TRIETHYL CITRATE

<https://www.femaflavor.org/flavor-library/triethyl-citrate>

## 20. FooDB

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<https://foodb.ca/about>

Triethyl citrate

<https://foodb.ca/compounds/FDB012587>

## 21. SpectraBase

Triethyl citrate

<https://spectrabase.com/spectrum/6WSLjjsviuR>

Triethyl citrate

<https://spectrabase.com/spectrum/4pAkq13fsQR>

TRIETHYL CITRATE

<https://spectrabase.com/spectrum/CIAh8xkFqI9>

TRIETHYL CITRATE

<https://spectrabase.com/spectrum/G0qqgVzbILR>

ETHYL CITRATE

<https://spectrabase.com/spectrum/7Zu1RzAQeYj>

TRIETHYL CITRATE

<https://spectrabase.com/spectrum/FGDFQJLx3I>

CITRIC ACID, TRIETHYL ESTER

<https://spectrabase.com/spectrum/9ALQETJSbZx>

Triethyl citrate

<https://spectrabase.com/spectrum/LnmYERKEweX>

Triethyl citrate

<https://spectrabase.com/spectrum/lt3L4Uom7z5>

Triethyl citrate

<https://spectrabase.com/spectrum/10nDpZCB9Ai>

Triethyl citrate

<https://spectrabase.com/spectrum/39z6mwQh2qD>

Triethyl citrate

<https://spectrabase.com/spectrum/359GkgPWGeU>

CITRIC ACID, TRIETHYL ESTER

<https://spectrabase.com/spectrum/EbF3NmZrEoh>

citric acid, triethyl ester

<https://spectrabase.com/spectrum/Dced9MGFDXI>

CITRIC ACID, TRIETHYL ESTER

<https://spectrabase.com/spectrum/CHIDL5gSEAK>

TRIETHYLCITRATE;TEC;94-025

<https://spectrabase.com/spectrum/GKU0nb1TcMW>

Citric acid, triethyl ester

<https://spectrabase.com/spectrum/Kzpc2e0sg5A>

CITRIC ACID, TRIETHYL ESTER

<https://spectrabase.com/spectrum/614hXkabWSQ>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/9u8jguthy7>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/4fySYA8zOnq>

1,2,3-PROPANETRICARBOXYLIC ACID, 2-HYDROXY-, TRIETHYL ESTER

<https://spectrabase.com/spectrum/HaBQ8YnuK3P>

1,2,3-PROPANETRICARBOXYLIC ACID, 2-HYDROXY-, TRIETHYL ESTER

<https://spectrabase.com/spectrum/8jzNmbwPovd>

Ethyl citrate

<https://spectrabase.com/spectrum/88zt0s1l0jDM>

Ethyl citrate

<https://spectrabase.com/spectrum/BAFwjhgntSa>

Ethyl citrate

<https://spectrabase.com/spectrum/7h5sFRS8Pge>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/6MxkU0t0a48>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/7e1Tb0ukWmm>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/jwKRn9nDYBc>

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<https://spectrabase.com/spectrum/1HZARan7K8e>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/HES0wHJhOiw>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/S1rvq9zYNNa>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/JUa3nwHgWjQ>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/4OKP4XjS72O>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/1l6kvM2Kydu>

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, triethyl ester

<https://spectrabase.com/spectrum/SyW1LiUr8vQ>

## 22. NIST Mass Spectrometry Data Center

Triethyl citrate

<http://www.nist.gov/srd/nist1a.cfm>

## 23. MassBank of North America (MoNA)

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<http://mona.fiehnlab.ucdavis.edu/spectra/browse?inchikey=DOOTYTYQINUNNV-UHFFFAOYSA-N>

## 24. NIPH Clinical Trials Search of Japan

<https://rctportal.niph.go.jp/en/>

## 25. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/341140608>

## 26. SpringerMaterials

2-hydroxy-propane-1,2,3-tricarboxylic acidtriethyl ester

[https://materials.springer.com/substanceprofile/docs/smsid\\_yjyxarnefeurdsxm](https://materials.springer.com/substanceprofile/docs/smsid_yjyxarnefeurdsxm)

## 27. Wikipedia

triethyl citrate

[https://en.wikipedia.org/wiki/Triethyl\\_citrate](https://en.wikipedia.org/wiki/Triethyl_citrate)

## 28. PubChem

<https://pubchem.ncbi.nlm.nih.gov>

## 29. MeSH

ethyl citrate

<https://www.ncbi.nlm.nih.gov/mesh/67023001>

## 30. Medical Subject Headings (MeSH)

MeSH Tree

<http://www.nlm.nih.gov/mesh/meshhome.html>

## 31. KEGG

Pharmaceutical additives in Japan

[http://www.genome.jp/kegg-bin/get\\_htext?br08316.keg](http://www.genome.jp/kegg-bin/get_htext?br08316.keg)

## 32. UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

GHS Classification Tree

[http://www.unece.org/trans/danger/publi/ghs/ghs\\_welcome\\_e.html](http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)

## 33. PATENTSCOPE (WIPO)

S/D 403386619

<https://pubchem.ncbi.nlm.nih.gov/substance/403386619>