



**COVID-19 is an emerging, rapidly evolving situation.**

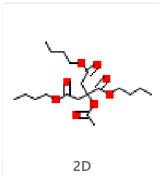
Get the latest public health information from CDC: <https://www.coronavirus.gov>.

Get the latest research from NIH: <https://www.nih.gov/coronavirus>.



## COMPOUND SUMMARY

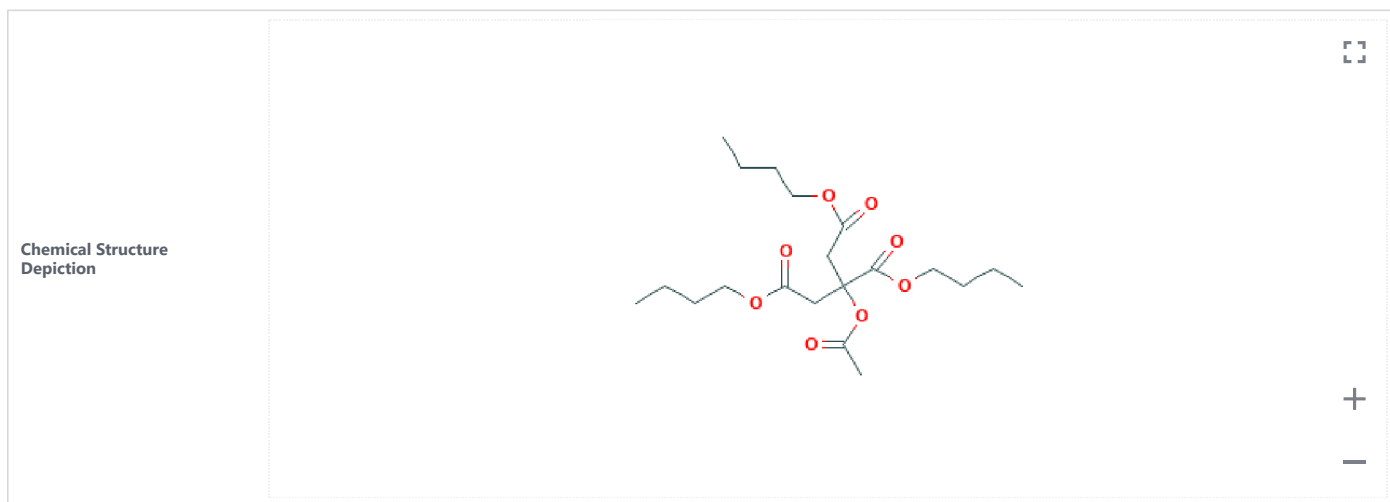
# Acetyl tributyl citrate

PubChem CID	6505
Structure	 2D <a href="#">Find Similar Structures</a>
Chemical Safety	<a href="#">Laboratory Chemical Safety Summary (LCSS) Datasheet</a>
Molecular Formula	C <sub>20</sub> H <sub>34</sub> O <sub>8</sub>
Synonyms	ACETYL TRIBUTYL CITRATE 77-90-7 tributyl 2-acetoxypropane-1,2,3-tricarboxylate Tributyl O-acetylcitrate Acetyltributyl citrate <input data-bbox="406 987 470 1018" type="button" value="More..."/>
Molecular Weight	402.5 g/mol
Dates	Modify    Create 2020-12-26    2005-03-26

# 1 Structures



## 1.1 2D Structure



► PubChem

## 1.2 3D Status



Conformer generation is disallowed since too flexible

► PubChem

## 2 Names and Identifiers

### 2.1 Computed Descriptors

#### 2.1.1 IUPAC Name

tributyl 2-acetyloxypropane-1,2,3-tricarboxylate

*Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)*

[▶ PubChem](#)

#### 2.1.2 InChI

InChI=1S/C20H34O8/c1-5-8-11-25-17(22)14-20(28-16(4)21,19(24)27-13-10-7-3)15-18(23)26-12-9-6-2/h5-15H2,1-4H3

*Computed by InChI 1.0.5 (PubChem release 2019.06.18)*

[▶ PubChem](#)

#### 2.1.3 InChI Key

QZCLKYGREBVARF-UHFFFAOYSA-N

*Computed by InChI 1.0.5 (PubChem release 2019.06.18)*

[▶ PubChem](#)

#### 2.1.4 Canonical SMILES

CCCCOC(=O)CC(CC(=O)OCCCC)(C(=O)OCCCC)OC(=O)C

*Computed by OEChem 2.1.5 (PubChem release 2019.06.18)*

[▶ PubChem](#)

### 2.2 Molecular Formula

C20H34O8

*Computed by PubChem 2.1 (PubChem release 2019.06.18)*

[▶ PubChem](#)

### 2.3 Other Identifiers

#### 2.3.1 CAS

77-90-7

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

#### 2.3.2 Deprecated CAS

37070-91-0, 791812-73-2

[▶ ChemIDplus](#)

#### 2.3.3 European Community (EC) Number

201-067-0

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

#### 2.3.4 NSC Number

3894

[▶ DTP/NCI](#)

## 2.3.5 UNII



0ZBX0N59RZ

[▶ FDA/SPL Indexing Data](#)

## 2.3.6 JECFA Number



630

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

## 2.3.7 FEMA Number



3080

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

## 2.3.8 DSSTox Substance ID



DTXSID2026446

[▶ EPA DSSTox](#)

## 2.3.9 Wikipedia

[Acetyl tributyl citrate](#)[▶ Wikipedia](#)

## 2.4 Synonyms



## 2.4.1 MeSH Entry Terms



2-acetyltributylcitrate  
 acetyl tributyl citrate  
 acetyltributylcitrate  
 ATBC plasticizer

[▶ MeSH](#)

## 2.4.2 Depositor-Supplied Synonyms



ACETYL TRIBUTYL CITRATE	ATBC	Acetyl butyl citrate	1,2,3-Propan
77-90-7	1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester	FEMA No. 3080	Citric acid, tri
tributyl 2-acetoxypropane-1,2,3-tricarboxylate	acetyltributylcitrate	tributyl 2-acetyloxypropane-1,2,3-tricarboxylate	DSSTox_CID
Tributyl O-acetylcitrate	Acetylcitric acid, tributyl ester	CCRIS 3409	DSSTox_RID
Acetyltributyl citrate	Tributyl acetylcitrate	HSDB 656	DSSTox_GSII
Tributyl acetylcitrate	Citric acid, tributyl ester, acetate	Tributyl 2-(acetyloxy)-1,2,3-propanetricarboxylate	Tributyl 2-(a
Citroflex A	Caswell No. 005AB	o-Acetylcitric acid tributyl ester	1,2,3-Propan
Blo-trol	UNII-0ZBX0N59RZ	2-Acetoxy-1,2,3-propanetricarboxylic acid tributyl ester	2-(Acetyloxy
Citroflex A 4	Acetyl tri-n-butyl citrate	EINECS 201-067-0	2-ACETYLOXY
Tributyl citrate acetate	NSC 3894	BRN 2303316	CAS-77-90-7
2-Acetyltributylcitrate	Uniplex 84	0ZBX0N59RZ	Acetyltribut
Tributyl acetyl citrate	Tributyl 2-acetoxy-1,2,3-propanetricarboxylate	AI3-01999	Estaflex

[▶ PubChem](#)

## 3 Chemical and Physical Properties



### 3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	402.5 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
XLogP3-AA	3.3	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	0	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	8	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	19	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	402.225368 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Monoisotopic Mass	402.225368 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Topological Polar Surface Area	105 Å <sup>2</sup>	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	28	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	476	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



DryPowder; Liquid

► [EPA Chemicals under the TSCA](#)

Liquid

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

colourless, slightly viscous liquid with very faint sweet herbaceous odour

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

### 3.2.2 Color/Form



Colorless liquid

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

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

### 3.2.3 Odor



Very faint sweet, herbaceous odor

*Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed. Boca Raton, FL 2005, p. 1817*

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

Odorless

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

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



### 3.2.4 Taste

At high levels (e.g., 1000 ppm emulsion in [water](#)) it has a mild, fruity, non-descript flavor.

*Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed. Boca Raton, FL 2005, p. 1817*

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

### 3.2.5 Boiling Point



331 °C at 732 mm Hg

*Oxea; OXBLUE ATBC, Acetyl Tributyl Citrate (CAS 77-90-7); Available from, as of June 15, 2015: <http://www.phthalate-free-plasticizers.com/acetyltributylcitrate-atbc.html>*

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

### 3.2.6 Melting Point



-80.0 °C

▶ [EPA DSSTox](#)

-80 °C

*Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 70*

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

-80°C

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

### 3.2.7 Flash Point



113 °C - closed cup

*GuideChem Safety Data Sheet: Tributyl O-acetylcitrate. Available from, as of December 11, 2015: <http://www.guidechem.com/msds/77-90-7.html>*

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

### 3.2.8 Solubility



1.24e-05 M

*CHEMICALS INSPECTION AND TESTING INSTITU (1992)*

▶ [EPA DSSTox](#)

In [water](#), 5 mg/L, temp not specified

*Chemicals Inspection and Testing Institute; Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chem Indus Ecol- Toxicol Informat Center. ISBN 4-89074-101-1 (1992)*

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

In [water](#), 4.49 mg/L at 20 °C

*Oxea; OXBLUE ATBC, Acetyl Tributyl Citrate (CAS 77-90-7); Available from, as of June 15, 2015: <http://www.phthalate-free-plasticizers.com/acetyltributylcitrate-atbc.html>*

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

In [water](#), 1.7 mg/L at 25 °C

*Yalkowsky, S.H., He, Yan, Jain, P. Handbook of Aqueous Solubility Data Second Edition. CRC Press, Boca Raton, FL 2010, p. 1239*

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

Soluble in organic solvents

*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: Aug 17, 2012.*

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

0.005 mg/mL

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

insoluble in [water](#); soluble in alcohol; miscible in oil

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

### 3.2.9 Density



1.046 at 25 °C

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

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

1.045-1.055

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

### 3.2.10 Vapor Density



14.1 (Air = 1; 20 °C)

*Oxea; OXBLUE ATBC, Acetyl Tributyl Citrate (CAS 77-90-7); Available from, as of June 15, 2015: <http://www.phthalate-free-plasticizers.com/acetyltributylcitrate-atbc.html>*

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

### 3.2.11 Vapor Pressure



3.0X10<sup>-4</sup> mm Hg at 25 °C (est)

*US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 15, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html>*

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

### 3.2.12 LogP



log Kow = 4.92

*US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2)*

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

### 3.2.13 Stability/Shelf Life



Stable under recommended storage conditions.

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

### 3.2.14 Decomposition



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

*Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3512*

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

### 3.2.15 Viscosity



42.7 cPs at 25 °C

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

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

### 3.2.16 Odor Threshold



Odor perception threshold is 50 mg/L.

*Sheftel, V.O.; Indirect Food Additives and Polymers. Migration and Toxicology. Lewis Publishers, Boca Raton, FL. 2000., p. 193*

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



### 3.2.17 Refractive Index

Index of refraction= 1.4408 at 25 °C

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

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

1.440-1.445

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

### 3.2.18 Kovats Retention Index



Standard non-polar	2253, 2224, 2253, 2253, 2224
Semi-standard non-polar	2250, 2254, 2221.2

▶ [NIST Mass Spectrometry Data Center](#)

### 3.2.19 Other Experimental Properties



VP: 1 mm Hg at 173 °C

Haynes, W.M. (ed.). *CRC Handbook of Chemistry and Physics. 95th Edition*. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-518

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

Distillation range: 172-174 °C (1 mm Hg); bulk density= 8.74 lb/gal (25 °C); combustible

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

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

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

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials. 12th Edition*. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 70

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

Boiling Point: 326 °C (purity not stated)

US EPA; *High Production Volume Information System (HPVIS)*. HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2)

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

Henry's Law constant = 3.8X10<sup>-10</sup> atm-cu m/mole at 25 °C /Estimated/

US EPA; *Estimation Program Interface (EPI) Suite*. Ver.3.11. June 10, 2003. Available from, as of Oct 27, 2004: <http://www.epa.gov/oppt/exposure/pubs/episutedl.htm>

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

Hydroxyl radical reaction rate constant = 1.4X10<sup>-11</sup> cu cm/molec-sec at 25 °C /Estimated/

US EPA; *Estimation Program Interface (EPI) Suite*. Ver.3.11. June 10, 2003. Available from, as of Oct 27, 2004: <http://www.epa.gov/oppt/exposure/pubs/episutedl.htm>

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



## 4 Spectral Information ? ↗

### 4.1 1D NMR Spectra ? ↗

**1D NMR Spectra** NMR: 10977 (Sadler Research Laboratories Spectral Collection)

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

**1D NMR Spectra** [1D NMR Spectrum 2633 - Acetyl tributyl citrate \(HMDB0034159\)](#)

[1D NMR Spectrum 3319 - Acetyl tributyl citrate \(HMDB0034159\)](#)

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

#### 4.1.1 1H NMR Spectra ? ↗

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

Thumbnail

▶ [SpectraBase](#)

<b>Instrument Name</b>	Varian A-60
<b>Copyright</b>	Copyright © 2009-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

▶ [SpectraBase](#)

#### 4.1.2 13C NMR Spectra ? ↗

<b>Source of Sample</b>	Chas. Pfizer & Company, Inc., New York, New York
<b>Copyright</b>	Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

[▶ SpectraBase](#)**Instrument Name** Varian HA-100**Copyright** Copyright © 2002-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.

Thumbnail

[▶ SpectraBase](#)

## 4.2 Mass Spectrometry

Showing 2 of 6 [View More](#) **Technique** GC/MS**Source of Spectrum** DigiLab GmbH (C) 2020**Copyright** Database Compilation Copyright © 2020 Wiley-VCH Verlag GmbH & Co. KGaA. Copyright © 2020 DigiLab GmbH. All Rights Reserved.

Thumbnail

► SpectraBase

<b>Source of Spectrum</b>	EP-2331-0-0
<b>Copyright</b>	Copyright © 2020 John Wiley & Sons, Inc. All Rights Reserved.
<b>Thumbnail</b>	

► SpectraBase

#### 4.2.1 GC-MS



Showing 2 of 7 [View More](#)

<b>GC-MS</b>	<a href="#">GC-MS Spectrum 27124 - Acetyl tributyl citrate (HMDB0034159)</a> <a href="#">GC-MS Spectrum 101530 - Acetyl tributyl citrate (HMDB0034159)</a>
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► [Human Metabolome Database \(HMDB\)](#)

<b>MoNA ID</b>	<a href="#">JP001729</a>
<b>MS Category</b>	Experimental
<b>MS Type</b>	GC-MS
<b>MS Level</b>	MS1
<b>Instrument</b>	Unknown
<b>Instrument Type</b>	CI-B
<b>Ionization Mode</b>	positive
<b>Splash</b>	<a href="#">splash10-0ufr-2159500000-62a9419892ec76844eb8</a>
<b>Thumbnail</b>	
<b>Submitter</b>	University of Tokyo Team, Faculty of Engineering, University of Tokyo

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

#### 4.2.2 LC-MS



Showing 2 of 5 [View More](#) 

MoNA ID	<a href="#">LU052301</a>
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H] <sup>+</sup>
precursor m/z	403.2326
Instrument	Q Exactive Orbitrap (Thermo Scientific)
Instrument Type	LC-ESI-QFT
Ionization	ESI
Ionization Mode	positive
Retention Time	19.698 min
Splash	<a href="#">splash10-05n0-0930000000-826c372828693a29286b</a>
Thumbnail	
Submitter	Anjana Elapavalore, Environmental Cheminformatics, LCSB, University of Luxembourg

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

MoNA ID	<a href="#">LU052302</a>
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H] <sup>+</sup>
precursor m/z	403.2326
Instrument	Q Exactive Orbitrap (Thermo Scientific)
Instrument Type	LC-ESI-QFT
Ionization	ESI
Ionization Mode	positive
Retention Time	19.698 min
Splash	<a href="#">splash10-0570-0900000000-7c9683615ce42b8ff890</a>
Thumbnail	

<b>Submitter</b>	Anjana Elapavalore, Environmental Cheminformatics, LCSB, University of Luxembourg
------------------	---

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

#### 4.2.3 EI-MS



<b>EI-MS</b>	<a href="#">EI-MS Spectrum 950 - Acetyl tributyl citrate (HMDB0034159)</a>
--------------	--

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

#### 4.2.4 Other MS



<b>Other MS</b>	MASS: 107140 (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: 6398 (Sadler Research Laboratories Prism Collection)
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► [Hazardous Substances Data Bank \(HSDB\)](#)

#### 4.3.1 FTIR Spectra



Showing 2 of 5 [View More](#)

<b>Technique</b>	BETWEEN SALTS
<b>Source of Sample</b>	Charles Pfizer & Company, Inc., New York, New York
<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>	Charles Pfizer & Company, Inc., New York, 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 3 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-107
<b>Lot Number</b>	080704001
<b>Copyright</b>	Copyright © 2012-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

► 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>	TCI Chemicals India Pvt. Ltd.
<b>Catalog Number</b>	A0822
<b>Copyright</b>	Copyright © 2016-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

► SpectraBase

### 4.3.3 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



<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>	TCI Chemicals India Pvt. Ltd.
<b>Catalog Number</b>	A0822
<b>Lot Number</b>	USBNC
<b>Copyright</b>	Copyright © 2016-2020 John Wiley & Sons, Inc. All Rights Reserved.
<b>Thumbnail</b>	

► SpectraBase

## 5 Related Records



### 5.1 Related Compounds with Annotation



▶ PubChem

## 5.2 Related Compounds



Same Connectivity	2 Records
Same Parent, Connectivity	5 Records
Same Parent, Exact	4 Records
Mixtures, Components, and Neutralized Forms	7 Records
Similar Compounds	216 Records

▶ PubChem

## 5.3 Substances



### 5.3.1 Related Substances



All	124 Records
Same	117 Records
Mixture	7 Records

▶ PubChem

### 5.3.2 Substances by Category





[▶ PubChem](#)

## 5.4 Entrez Crosslinks



PubMed	<a href="#">19 Records</a>
Taxonomy	<a href="#">5 Records</a>
Gene	<a href="#">14 Records</a>

[▶ PubChem](#)

## 6 Chemical Vendors

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▶ PubChem

## 7 Food Additives and Ingredients



### 7.1 Food Additive Classes



#### Flavoring Agents

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

#### JECFA Functional Classes

Flavoring Agents -> FLAVOURING\_AGENT

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

### 7.2 FEMA Flavor Profile



#### Floral

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

### 7.3 FDA Substances Added to Food



Substance	<a href="#">TRIBUTYL ACETYLCITRATE</a>
Used for (Technical Effect)	FLAVORING AGENT OR ADJUVANT
Document Number (21 CFR)	<a href="#">172.515</a> <a href="#">175.105</a> <a href="#">175.300</a> <a href="#">175.320</a> <a href="#">178.3910</a> <a href="#">181.27</a>

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

### 7.4 Organoleptic Properties



#### Flavors

[wine](#)  
[sweet](#)  
[herbal](#)  
[very faint](#)

- ▶ [FooDB](#)

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



Chemical Name	ACETYL TRIBUTYL CITRATE
Evaluation Year	1999
ADI	No safety concern at current levels of intake when used as a flavouring agent
Report	<a href="#">TRS 896-JECFA 53/67</a>

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

## 8 Pharmacology and Biochemistry



### 8.1 Absorption, Distribution and Excretion



The metabolism of acetyl tributyl citrate was evaluated using groups of male rats (number of animals, weights, and strain not stated). Each animal received a single oral dose of <sup>14</sup>C-acetyl tributyl citrate (dose not stated). At 48 hr post dosing, approximately 99% of the administered dose had been excreted either in urine (59% to 70%), feces (25% to 36%), or in the expired air (2%). Only 0.36% to 1.26% of the dose remained in the tissues or carcass.

*Johnson W; International Journal of Toxicology 21 (Suppl.2): 1-17 (2002)*

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

### 8.2 Metabolism/Metabolites



The metabolism of acetyl tributyl citrate was evaluated using groups of male rats (number of animals, weights, and strain not stated). ... Both the absorption and metabolism of <sup>14</sup>C-Acetyl tributyl Citrate proceeded rapidly, and the following metabolites were identified: [acetyl citrate](#), monobutyl citrate, acetyl monobutyl citrate, dibutyl citrate, and acetyl dibutyl citrate.

*Johnson W; International Journal of Toxicology 21 (Suppl.2): 1-17 (2002)*

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

### 8.3 Human Metabolite Information



#### 8.3.1 Cellular Locations



Membrane

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

## 9 Use and Manufacturing



### 9.1 Overview



**IDENTIFICATION:** Acetyl tributyl citrate is a colorless liquid. It has a very faint sweet, herb-like odor and a mild fruity taste. Acetyl tributyl citrate has moderate solubility in [water](#). **USE:** Acetyl tributyl citrate is an important commercial chemical that is used as a solvent in paints, inks, and nail enamel. It is also used to make plastics more flexible, including plastics used to make toys and food wrappings. Acetyl tributyl citrate is added as a flavor ingredient in non-alcoholic beverages and is used in the manufacture of many pharmaceutical drugs. **EXPOSURE:** Workers that use or produce acetyl tributyl citrate may breathe in mists or have direct skin contact. The general population may be exposed to small amounts by drinking beverages containing acetyl tributyl citrate, eating foods stored in plastic materials containing acetyl tributyl citrate, or from skin contact with products containing acetyl tributyl citrate. If acetyl tributyl citrate is released to air, it will be broken down by reaction with other chemicals. It will be in or on particles that eventually fall to the ground. If released to [water](#) or soil, acetyl tributyl citrate is expected to bind to soil particles or suspended particles. Acetyl tributyl citrate is not expected to move through soil. Acetyl tributyl citrate is expected to move into air from wet soils or [water](#) surfaces. However, binding to soil may slow down this process. Acetyl tributyl citrate is expected to be broken down by microorganisms and may have moderate build up in tissues of aquatic organisms. **RISK:** Acetyl tributyl citrate did not cause skin irritation or allergic reactions in human volunteers. Additional information about the potential for acetyl tributyl citrate to produce toxic effects in humans was not located. Very mild to no skin irritation and moderate eye irritation have been reported in laboratory animals. No toxic effects were observed in laboratory animals given a single high oral dose of acetyl tributyl citrate. Diarrhea, weight loss, and liver damage were observed in laboratory animals repeatedly fed very high doses. Body weight loss was observed in laboratory animals following repeated skin application of high levels of acetyl tributyl citrate. No changes were observed in reproduction or development in rats exposed to high dose over a short period of time. No tumors were reported in laboratory animals following life-time exposure to high dietary levels of acetyl tributyl citrate. The potential for acetyl tributyl 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 23, 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 23, 2015: <http://monographs.iarc.fr/ENG/Classification/index.php> (3) National Library of Medicine Household Products Database. Available from, as of Jun 23, 2015: <http://hpd.nlm.nih.gov/> (4) National Toxicology Program. Nomination Summary for Acetyl tributyl citrate (ATBC) RTP No. N91007. Available from, as of Jun 23, 2015: <http://ntp.niehs.nih.gov/> (5) National Toxicology Program. Thirteenth Report on Carcinogens. Available from, as of Jun 23, 2015: <http://ntp.niehs.nih.gov/pubhealth/roc/index.html> (6) US EPA; High Production Volume Information System (HPVIS). 1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester. 77-90-7. Available from, as of Jun 23, 2015: <http://www.epa.gov/hpv/hpvis/index.html> (7) USEPA; HPV Chemical Characterizations. 1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester (77-90-7) Sept 2014. Available from, as of Jun 23, 2015: [http://iaspub.epa.gov/opphpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opphpv/hpv_hc_characterization.get_report?doctype=2) (8) USEPA/IRIS Integrated Risk Information System. Available from, as of Jun 23, 2015: <http://www.epa.gov/iris/> (9) US FDA. Everything Added to Food in the United States (EAFUS). November 2011. Tributyl acetyl citrate. Available from, as of Jun 23, 2015: <http://www.accessdata.fda.gov/scripts/fcn/fcnNavigation.cfm?rpt=eafusListing>

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

### 9.2 Use Classification



Food additives -> Flavoring Agents

▶ [EU Food Improvement Agents](#)

Flavoring Agents -> FLAVOURING\_AGENT -> 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 -> Film forming; Plasticiser

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](#)

### 9.3 Uses



EPA CPDat Chemical and Product Categories

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

#### Plasticizer for vinyl resins

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

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

#### Plasticizer (rubber, cellulosic resins)

*Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 902*

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

... Use in the production of food-contact surfaces of resinous and polymeric coatings and in paper/paperboard for use in contact with fatty foods.

*Sheftel, V.O.; Indirect Food Additives and Polymers. Migration and Toxicology. Lewis Publishers, Boca Raton, FL. 2000., p. 193*

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

... /the most widely used phtahalate substitute plasticizer/ widely used in products such as food wrap, vinyl toys, and pharmaceutical excipients ...

[PMID:21742782](#)

*Takeshita A et al; Toxicol Sci 123 (2): 460-70 (2011)*

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

...the most widely used phtahalate substitute plasticizer...

[PMID:21742782](#)

*Takeshita A et al; Toxicol Sci 123 (2): 460-70 (2011)*

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

It is used as a plasticizer for [cellulose nitrate](#), [cellulose acetate](#), and [polyvinyl acetate](#) ... also used in cosmetics.

*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: Aug 17, 2012.*

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

Non-confidential information in the IUR /Information Update Rule/ indicated that the industrial processing and uses of the chemical include other basic organic chemical manufacturing as corrosion inhibitors and antiscaling agents and functional fluids; resin and synthetic rubber manufacturing, and other chemical and allied products merchant wholesalers as functional fluids; adhesive manufacturing, other basic inorganic chemical manufacturing, other plastic product manufacturing, paints and coating manufacturing, pharmaceutical and medicine manufacturing, plastic packaging materials and unlaminated film and sheet manufacturing, and paint ink manufacturing as "other." Nonconfidential commercial and consumer uses of this chemical include metal products, rubber and plastic products and "other."

*US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opphpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opphpv/hpv_hc_characterization.get_report?doctype=2)*

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

#### Reported uses (ppm):

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

Food Category	Usual	Max.
Nonalcoholic beverages	1.00	1.00

*Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed. Boca Raton, FL 2010, p. 1927*

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

### 9.3.1 Industry Uses



Intermediates  
Paint additives and coating additives not described by other categories  
Pigments  
Plasticizers  
Processing aids, not otherwise listed

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

► [EPA Chemicals under the TSCA](#)

### 9.3.2 Consumer Uses



Adhesives and sealants

Automotive care products  
Ink, toner, and colorant products  
Non-TSCA use  
Plastic and rubber products not covered elsewhere

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

▶ [EPA Chemicals under the TSCA](#)

## 9.4 Methods of Manufacturing



From [citric acid](#) via the tributyl ester followed by acetylation.

*Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed. Boca Raton, FL 2010, p. 1927*

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

## 9.5 Formulations/Preparations



Grade: Technical

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

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

## 9.6 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](#)

(1976) GREATER THAN 2X10+6 GRAMS

*SRI*

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

[1,2,3-Propanetricarboxylic acid](#), 2-(acetyloxy)-, tributyl ester is listed as a High Production Volume (HPV) chemical (65FR81686). Chemicals listed as HPV were produced in or imported into the U.S. in >1 million pounds in 1990 and/or 1994. The HPV list is based on the 1990 Inventory Update Rule. (IUR) (40 CFR part 710 subpart B; 51FR21438).

*EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program. 1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester (77-90-7). Available from, as of June 30, 2015: <http://www.epa.gov/hpv/pubs/general/opptsrch.htm>*

▶ [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-(acetyloxy)-, 1,2,3-tributyl ester. National Production Volume: 4,669,244 lb/yr.

*USEPA/Pollution Prevention and Toxics; 2012 Chemical Data Reporting Database. 1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, 1,2,3-tributyl ester (77-90-7). Available from, as of June 30, 2015: [http://java.epa.gov/oppt\\_chemical\\_search/](http://java.epa.gov/oppt_chemical_search/)*

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

## 9.7 General Manufacturing Information



Industry Processing Sectors

Adhesive manufacturing  
All other basic inorganic chemical manufacturing  
All other basic organic chemical manufacturing  
All other chemical product and preparation manufacturing  
Custom compounding of purchased resin  
Paint and coating manufacturing  
Pharmaceutical and medicine manufacturing  
Plastic material and resin manufacturing  
Plastics product manufacturing  
Printing ink manufacturing

▶ [EPA Chemicals under the TSCA](#)

EPA TSCA Commercial Activity Status

1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, 1,2,3-tributyl ester: ACTIVE

<https://www.epa.gov/tsca-inventory>

▶ [EPA Chemicals under the TSCA](#)



## 10 Safety and Hazards



### 10.1 Hazards Identification



#### 10.1.1 GHS Classification



<b>GHS Hazard Statements</b>	Not Classified Reported as not meeting GHS hazard criteria by 2035 of 2064 companies (only ~ 1.4% companies provided GHS information). For more detailed information, please visit <a href="#">ECHA C&amp;L website</a> .
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▶ [European Chemicals Agency \(ECHA\)](#)

### 10.2 Fire Fighting



#### 10.2.1 Fire Fighting Procedures



Wear self contained breathing apparatus for fire fighting if necessary.

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

Use [water](#) spray, alcohol-resistant foam, dry chemical or [carbon dioxide](#).

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

### 10.3 Accidental Release Measures



#### 10.3.1 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; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

#### 10.3.2 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; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

#### 10.3.3 Preventive Measures



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

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 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; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

## 10.4 Handling and Storage



### 10.4.1 Storage Conditions



Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Moisture sensitive.

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

## 10.5 Exposure Control and Personal Protection



### 10.5.1 Allowable Tolerances



Residues resulting from the use of the following substances as either an inert or an active ingredient in a pesticide chemical formulation, including antimicrobial pesticide chemicals, are 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, 2-(acetyloxy)-, tributyl ester** is included on this list.

*40 CFR 180.950(e) (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 29, 2015: <http://www.ecfr.gov>*

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

### 10.5.2 Personal Protective Equipment (PPE)



Skin protection: Handle with gloves.

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

Eye/face protection: Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 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; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

Body Protection: Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

## 10.6 Stability and Reactivity



### 10.6.1 Hazardous Reactivities and Incompatibilities



Strong oxidizing agents

*Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>*

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

## 10.7 Regulatory Information

### 10.7.1 FIFRA Requirements

Residues resulting from the use of the following substances as either an inert or an active ingredient in a pesticide chemical formulation, including antimicrobial pesticide chemicals, are 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, 2-(acetyloxy)-, tributyl ester** is included on this list.

40 CFR 180.950(e) (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of November 1, 2004: <http://www.ecfr.gov>

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

### 10.7.2 FDA Requirements

Food additive permitted for direct addition to food for human consumption as a synthetic flavoring substance and adjuvant in accordance with the following conditions: a) they are used in the minimum quantity required to produce their intended effect, and otherwise in accordance with all the principles of good manufacturing practice, and b) they consist of one or more of the following, used alone or in combination with flavoring substances and adjuvants generally recognized as safe in food, prior-sanctioned for such use, or regulated by an appropriate section in this part. Tributyl acetylcitrate is included on this list.

21 CFR 172.515 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of July 1, 2015: <http://www.ecfr.gov>

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

Acetyl tributyl citrate is an indirect food additive for use only as a component of adhesives.

21 CFR 175.105 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 29, 2015: <http://www.ecfr.gov>

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

Prior-sanctioned food ingredients. Substances classified as plasticizers, when migrating from food packaging material. Acetyl tributyl citrate is included on this list.

21 CFR 181.27 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 29, 2015: <http://www.ecfr.gov>

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

## 10.8 Other Safety Information

### 10.8.1 Toxic Combustion Products

Carbon oxides

Sigma-Aldrich; Safety Data Sheet for Tributyl O-acetylcitrate. Product Number: 388378, Version 5.3 (Revision Date 07/01/2014). Available from, as of May 28, 2015: <http://www.sigmaaldrich.com/safety-center.html>

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

### 10.8.2 Special Reports

The U.S. high production volume (HPV) chemicals are those which are manufactured in or imported into the United States in amounts equal to or greater than one million pounds per year. Robust Summaries include health effects, ecotoxicity data, and environmental fate information for selected chemicals. EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans.[Available from, as of November 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>]

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

## 11 Toxicity



### 11.1 Toxicological Information



#### 11.1.1 Acute Effects



► [ChemiDplus](#)

#### 11.1.2 Toxicity Summary



**IDENTIFICATION AND USE:** Acetyl tributyl citrate (ATBC) is a colorless liquid. It is the most widely used [phthalate](#) substitute plasticizer. It is used in products such as food wrap, vinyl toys, and pharmaceutical excipients. It is also used as a flavor ingredient in non-alcoholic beverages. **HUMAN EXPOSURE AND TOXICITY:** The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women, all of whom had history of diabetes, psoriasis, or active dermatoses. ATBC was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study. In vitro ATBC increased CYP3A4 messenger RNA (mRNA) levels and enzyme activity in the human intestinal cells but not in human liver cells. **ANIMAL STUDIES:** Acute oral toxicity of ATBC in cats and rats is low. CYP3A1 mRNA levels were increased in the intestine but not the liver of ATBC-treated rats. In a 90-day repeated-dose oral dietary study in rats, decreased body weight and organ weight changes were observed at 1000 mg/kg-bw/day. In a combined repeated dose/reproductive/developmental toxicity study in rats, organ weight and histopathological changes were observed in adults at 1000 mg/kg-bw/day. In a 2-generation reproductive toxicity study in rats, reduced body weight was observed in F1 males at 300 mg/kg-bw/day. In the same study, no other treatment related effects were observed. In the combined repeated dose/reproductive/developmental toxicity study in rats previously described, histopathological changes were observed in the liver of adult males at 300 mg/kg-bw/day. In the same study, decreased litter size and decreased number of implantations were observed at 1000 mg/kg-bw/day. ATBC did not induce gene mutations in bacteria or mammalian cells in vitro and did not induce chromosomal aberrations in mammalian cells in vitro. **ECOTOXICITY STUDIES:** For acetyl tributyl citrate, the 96-hr LC50 values for fish range from 38 to 60 mg/L, the 48-hr EC50 value for aquatic invertebrates is 7.8 mg/L and the 72-hr EC50 values for aquatic plants are 11.5 mg/L for biomass and 74.4mg/L for growth rate, respectively.

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

#### 11.1.3 Antidote and Emergency Treatment



**/SRP:/** 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 if necessary. Immediately flush contaminated eyes with gently flowing [water](#). Do not induce vomiting. If vomiting occurs, lean patient forward or place on the 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. **/Poisons A and B/**

*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. 160*

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

**/SRP:/** 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 needed. Administer [oxygen](#) by nonbreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if necessary ... . Anticipate seizures 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 ... . Cover skin burns with dry sterile dressings after decontamination ... . **/Poisons A and B/**

*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. 160*

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

**/SRP:/** 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 ... . Consider administering a beta agonist such as [albuterol](#) for severe bronchospasm ... . Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start IV

administration of 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. Watch for signs of fluid overload ... . Treat seizures with [diazepam](#) or [lorazepam](#) ... . Use [proparacaine hydrochloride](#) to assist eye irrigation ... . /Poisons A and B/

*Currance, P.L. Clements, B., Bronstein, A.C. (Eds.); Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160-1*

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

### 11.1.4 Human Toxicity Excerpts



/HUMAN EXPOSURE STUDIES/ The skin irritation potential of acetyl tributyl citrate was evaluated using 59 men and women (age range = 21-60 years), all of whom had history of diabetes, psoriasis, or active dermatoses. ... Occlusive patches moistened with 0.4 mL of acetyl tributyl citrate were applied to the upper arm of each subject on Mondays, Wednesdays, and Fridays for 3 consecutive weeks. Each patch was removed 24 hours post application. Induction reactions were scored prior to patch applications (second through ninth visits) and at the time of the tenth visit. Duplicate challenge of the test material was made after a two-week non-treatment period. ... One challenge patch was applied to the original test site, and , another, to an adjacent site. Challenge reactions were scored at 48 and 96 hours post application. /Acetyl tributyl citrate/ was nonirritating to the skin, and reactions suggestive of contact sensitization were not observed during the study.

*Johnson W; International Journal of Toxicology 21 (Suppl.2): 1-17 (2002)*

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

/ALTERNATIVE and IN VITRO TESTS/ The cytotoxicity of acetyl-tributyl-citrate and [dibutyl-sebacate](#) was studied in cultured mammalian cells. The impetus for the study was a report that acetyl-tributyl-citrate and [dibutyl-sebacate](#), which were plasticizers found in [polyvinylidene-chloride](#) film used for packaging food, could leach out and diffuse into the foods. Human KB cells, monkey Vero cells, and canine MDCK cells were incubated with acetyl-tributyl-citrate or [dibutyl sebacate](#) over a range of concentrations for 72 hours. Cytotoxicity was evaluated by determining the extent of growth inhibition. Doses of acetyl-tributyl-citrate and [dibutyl-sebacate](#) that inhibited growth by 50% were calculated from the data. Both compounds inhibited the growth of all cells in a dose dependent manner. The inhibited growth by 50% of acetyl-tributyl-citrate in the various types were: 44.7 ug/mL in KB cells; 39.9 ug/mL in Vero cells; and 42.1 ug/mL in MDCK cells. The inhibited growth by 50% of [dibutyl-sebacate](#) in these cells were: KB cells, 1,549 ug/mL; Vero cells, 1,510 ug/mL; and MDCK cells, 1,549 ug/mL. /It was/ concluded that when comparing the results of this study with those obtained previously using [tricesyl-phosphate](#), [triphenyl-phosphate](#) (TPP), butylated-hydroxyanisole, and butylated-hydroxytoluene in human KB cells, acetyl-tributyl-citrate is more toxic than TCP and more toxic than TPP. Acetyl-tributyl-citrate is less toxic than BHA, but shows toxicity similar to that of BHT. DBS is much less toxic than either BHT or BHA. KB, Vero, and MDCK cells show similar sensitivity to acetyl-tributyl-citrate and DBS.

[PMID:8645922](#)

*Mochida K et al; Bulletin of Environmental Contamination and Toxicology 56 (4): 635-7 (1996)*

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

/ALTERNATIVE and IN VITRO TESTS/ The in vitro cytotoxicity of acetyl tributyl citrate in HeLa cell cultures (human cell line) was evaluated using the metabolic inhibition test, supplemented by microscopy of cells after 24 hours of incubation (the MIT-24 test system). ... After 24 hours, cell viability was determined by microscopy. Two endpoints of cytoinhibition (total and partial inhibition) were estimated after 24 hours, based on the absence or scarcity of spindle-shaped cells, and, after 7 days.... The following values for minimal inhibitory concentration were reported for acetyl tributyl citrate: 13 mg/mL (for total inhibition at 24 hours), 3.8 mg/mL (for partial inhibition at 24 hours), and 5.7 mg/mL (for total and partial inhibition at 7 days). Acetyl tributyl citrate caused little toxicity in HeLa cell cultures.

*Johnson W; International Journal of Toxicology 21 (Suppl.2): 1-17 (2002)*

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

/ALTERNATIVE and IN VITRO TESTS/ The effects of polyvinyl-[chloride](#) (PVC) tubing extracts were investigated in isolated ileum of guinea-pigs. Ileum were isolated and mounted in tissue baths. Tubing ingredients from PVC or tubing extracts of the plasticizer acetyl-N-tributyl-citrate (ATBC) were added to the bath for 15 minutes. Contractions or modifications of [methacholine](#) responses were measured. ...A significant and characteristic effect was seen for ATBC in ileum, consisting of rapid contractions and relaxations which were dependent on concentrations. The spasms were unaffected by [tetrodotoxin](#). No spasmogenic effect was seen for ATBC in human small intestine or colon. None of the other tubing ingredients had any spasmogenic action, including PVC extracts. No [methacholine](#) contractions occurred with the other ingredients. Tubing extracts containing ATBC produced spasms similar to chemical ATBC.

*Hollingsworth M; J Biomed Mat Res 9 (6): 687-97 (1975)*

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

/ALTERNATIVE and IN VITRO TESTS/ Steroid and xenobiotic receptor (SXR) is activated by endogenous and exogenous chemicals including steroids, bile acids, and prescription drugs. SXR is highly expressed in the liver and intestine, where it regulates cytochrome P450 3A4 (CYP3A4), which in turn controls xenobiotic and endogenous steroid hormone metabolism. However, it is unclear whether Food and Drug Administration (FDA)-approved plasticizers exert such activity. ...We found that four of eight FDA-approved plasticizers increased SXR-mediated transcription. In particular, acetyl tributyl citrate (ATBC), an industrial plasticizer widely used in products such as food wrap, vinyl toys, and pharmaceutical excipients, strongly activated human and rat SXR. ATBC increased CYP3A4 messenger RNA (mRNA) levels and enzyme activity in the human intestinal cells but not in human liver cells.

[PMID:21742782](#)

*Takeshita A et al; Toxicol Sci 123 (2): 460-70 (2011)*

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

### 11.1.5 Non-Human Toxicity Excerpts



/LABORATORY ANIMALS: Acute Exposure/ The intravenous administration of acetyl tributyl citrate to cats and rabbits induced a dose-related decrease in blood pressure. /Acetyl tributyl citrate/ caused complete loss of blood pressure when administered in toxic doses. The results of experiments conducted on the isolated rabbit heart indicate that this effect on blood pressure was due to cardiac inhibition.

Johnson W; *International Journal of Toxicology* 21 (Suppl.2): 1-17 (2002)

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

/LABORATORY ANIMALS: Acute Exposure/ In both rats and cats ... single oral doses of 10-30 mL/kg of tributyl acetylcitrate did not produce marked effects on the animals.

Lefaux, R. *Practical Toxicology of Plastics*. Cleveland: CRC Press Inc., 1968., p. 369

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

/LABORATORY ANIMALS: Acute Exposure/ The acute oral toxicity of Acetyl tributyl citrate was evaluated using five rats (strain and weight not stated). The test substance was administered at doses ranging from 10 to 30 mL/kg, and animals were observed for 3 weeks. Signs of systemic toxicity were not observed, and none of the animals died.

Johnson W; *International Journal of Toxicology* 21 (Suppl.2): 1-17 (2002)

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

/LABORATORY ANIMALS: Acute Exposure/ A single dose of acetyl tributyl citrate (30 to 50 mL/kg) was administered by stomach tube to each of four fasted cats (weights not stated), and animals were observed for 2 months. Two additional cats served as controls. Signs of nausea were observed in test animals, and, within a few hours of dosing, diarrhea (oozing of oily material) was noted. The diarrhea subsided within 24 hours of dosing. The behavior and general appearance of animals indicated systemic toxicity. Two cats dosed with 50 mL/kg were used for hematological evaluations and no effects on the following blood parameters were found: blood cell counts, hemoglobin, sugar, nonprotein **nitrogen**, or **creatinine**. Results from urinalyses indicate no abnormalities in specific gravity, albumin, sugar, pH, or microscopic formed elements.

Johnson W; *International Journal of Toxicology* 21 (Suppl.2): 1-17 (2002)

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

For more Non-Human Toxicity Excerpts (Complete) data for ACETYL TRIBUTYL CITRATE (23 total), please visit the [HSDB record page](#).

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

## 11.1.6 Non-Human Toxicity Values



### LD50 Rat oral 31.4 g/kg

Sheftel, V.O.; *Indirect Food Additives and Polymers. Migration and Toxicology*. Lewis Publishers, Boca Raton, FL. 2000., p. 193

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

### LD50 Mouse ip >4 g/kg

Lewis, R.J. Sr. (ed) *Sax's Dangerous Properties of Industrial Materials*. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3512

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

### LD50 Cat oral >50 mL/kg

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Acetyltributyl Citrate. Available from, as of May 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>

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

## 11.1.7 Ecotoxicity Values



LC50; Species: *Fundulus heteroclitus* (Mummichogs) length 3.5-8.5 in; Conditions: flow through tanks delivered 4.8 volume replacements/day; the dilution **water** was synthetic seawater (25%); the pH ranged from 6.5-7.6; the dissolved **oxygen** concentration was 70-95% saturation; temperature was maintained at approximately 23-24 °C; Concentration: 59 mg/L for 96 hr.

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Acetyltributyl Citrate. Available from, as of May 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>

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

LC50; Species: *Lepomis macrochirus* (Bluegill sunfish); Conditions: flow through tanks delivered 4.8 volume replacements/day; the pH ranged from 6.5-7.6; the dissolved **oxygen** concentration was 70-95% saturation; temperature was maintained at approximately 23-24 °C; Concentration: 38-60 mg/L for 96 hr.

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Acetyltributyl Citrate. Available from, as of May 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>

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

LC50; Species: *Pimephales promelas* (Fathead minnow) 18-hr old larval fish; Conditions: static renewal, total hardness and alkalinity ranges of 150 mg/L and 152 mg/L as CaCO<sub>3</sub>, respectively; specific conductance of 332 uS/cm, temperature in the test solutions ranged from 24.5-25.3 °C, dissolved **oxygen** concentrations ranged from 7.4-8.45 in fresh solutions and 4.9-7.13 mg/L in expired solutions, pH ranged from 7.69-8.27 in fresh solutions and from 7.61-8.23 in expired solutions; Concentration:

3.5 mg/L for 24 hr (95% confidence interval: 3.4-3.7 mg/L), 2.8 mg/L for 48 hr (95% confidence interval: 2.5-3.2 mg/L), 1.9 mg/L for 7 days (95% confidence interval: 1.8-2.1 mg/L)

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Acetyltributyl Citrate. Available from, as of May 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>

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

EC50; Species: Pimephales promelas (Fathead minnow) 18-hr old larval fish; Conditions: static renewal; total hardness and alkalinity ranges of 150 mg/L and 152 mg/L as CaCO<sub>3</sub>, respectively; specific conductance of 332 uS/cm; temperature in the test solutions ranged from 24.5-25.3 °C; dissolved oxygen concentrations ranged from 7.4-8.45 in fresh solutions and 4.9-7.13 mg/L in expired solutions; pH ranged from 7.69-8.27 in fresh solutions and from 7.61-8.23 in expired solutions; Concentration: 1.4 mg/L for 7 days (95% confidence interval: 0.72-2.7 mg/L); Effect: reduced growth

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Acetyltributyl Citrate. Available from, as of May 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>

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

EC50; Species: Ceriodaphnia dubia (Water flea); Conditions: static, temperature was maintained at 25+/-2 °C, dissolved oxygen concentrations ranged from 6.99-8.03 mg/L, pH ranged from 7.46-8.34, hardness was 154 mg/L as CaCO<sub>3</sub>, alkalinity was 156 mg/L as CaCO<sub>3</sub>, and conductivity was 337 uS/cm; Concentration: 7.82 mg/L for 48 hr; Effect: percent immobilization

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Acetyltributyl Citrate. Available from, as of May 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>

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

## 11.1.8 Ecotoxicity Excerpts



/AQUATIC SPECIES/ The study measured the acute toxicity of the test substance to locally obtained bluegill sunfish during a 96-hr exposure period in flow-through systems. Fish were acclimated to laboratory conditions for >1 month before use in this study. Following 96-hr exposure, observation for mortality and behavioral effects were monitored for an additional 96 hours. Experimental conditions during this study were as follows: flow through tanks delivered 4.8 volume replacements/day; the pH ranged from 6.5-7.6; the dissolved oxygen concentration was 70-95% saturation; temperature was maintained at approximately 23-24 °C; and fish were not fed during the first 96 hours of an extended exposure period. ...The fish exposed to low concentrations of the test substance appeared to be more excitable than usual, while activity was greatly reduced in fish exposed to the higher concentrations. Loss of equilibrium was observed and, at higher concentrations, a marked loss of equilibrium and fine fin movements was observed. Gill motion was irregular and shallow. All fish reportedly recovered from treatment-related effects within 48 hours of cessation of exposure to the test substance.

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Acetyltributyl Citrate. Available from, as of May 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>

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

/AQUATIC SPECIES/ The study measured the acute toxicity of the test substance to locally obtained mummichogs during a 96-hr exposure period in flow-through tanks. Fish were acclimated to laboratory conditions for several weeks before use in this study. Following 96-hr exposure, observation for mortality and behavioral effects were monitored for an additional 96 hours. Experimental conditions during this study were as follows: flow through tanks delivered 4.8 volume replacements/day; the dilution water was synthetic seawater (25%); the pH ranged from 6.5-7.6; the dissolved oxygen concentration was 70-95% saturation; temperature was maintained at approximately 23-24 °C; and fish were not fed during the first 96 hours of an extended exposure period. Mummichogs were 3.5-8.5 inches in length. ...Behavioral effects were observed in fish exposed to 50 mg/L of the test substance in <48 hours. Some survival was seen at 100 mg/L after 96 hours of exposure. The fish exposed to low concentrations of the test substance appeared to be more excitable than usual, while activity was greatly reduced in fish exposed to the higher concentrations. Loss of equilibrium was observed and, at higher concentrations, a marked loss of equilibrium and fine fin movements (especially pectoral fins) was observed. Gill motion was irregular and shallow. ... Two severely affected fish were transferred from test solutions to fresh water, one of which fully recovered from exposure to a 120 mg/L test solution for 7.5 hours and the other recovered from exposure to an 80 mg/L test solution after 24 hours. All surviving fish reportedly recovered from treatment-related effects within 48 hours of cessation of exposure to the test substance. /Citroflex-A4 (O-acetyl-tributyl citrate)/

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program's Robust Summaries and Test Plans. Acetyltributyl Citrate. Available from, as of May 28, 2015: <http://www.epa.gov/hpv/pubs/hpvrstp.htm>

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

## 11.1.9 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 \(HSDB\)](#)

## 11.2 Ecological Information



### 11.2.1 Environmental Fate/Exposure Summary





Acetyl tributyl citrate's production and use as a plasticizer for vinyl and other resins, as a solvent and functional fluid in adhesives, paints, coating and inks and as a flavor ingredient may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of  $3 \times 10^{-4}$  mm Hg at 25 °C indicates acetyl tributyl citrate will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase acetyl tributyl 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 27 hours. Particulate-phase acetyl tributyl citrate will be removed from the atmosphere by wet and dry deposition. If released to soil, acetyl tributyl citrate is expected to have slight mobility based upon an estimated Koc of 3,280. Volatilization from moist soil surfaces is expected to be an important fate process based upon an estimated Henry's Law constant of  $3.2 \times 10^{-5}$  atm-cu m/mole. However, adsorption to soil is expected to attenuate volatilization. Acetyl tributyl citrate is not expected to volatilize from dry soil surfaces based upon its estimated vapor pressure. Utilizing the Japanese MITI test, 82% of the Theoretical BOD was reached in 4 weeks indicating that biodegradation is an important environmental fate process in soil and [water](#). Two soil degradation studies observed rapid biomineralization of acetyl tributyl citrate. If released into [water](#), acetyl tributyl citrate is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Acetyl tributyl citrate has been shown to biodegrade extensively in several other biodegradation studies and simulation tests. Volatilization from [water](#) surfaces is expected to be an important fate process based upon this compound's estimated Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 2.6 and 25 days, respectively. However, volatilization from [water](#) surfaces is expected to be attenuated by adsorption to suspended solids and sediment in the [water](#) column. The estimated volatilization half-life from a model pond is 335 days if adsorption is considered. An estimated BCF of 35 suggests the potential for bioconcentration in aquatic organisms is moderate. Estimated hydrolysis half-lives of 3.8 years and 140 days were determined for pH 7 and 8, respectively. Occupational exposure to acetyl tributyl citrate may occur through inhalation and dermal contact with this compound at workplaces where acetyl tributyl citrate is produced or used. Use data indicate that the general population may be exposed to acetyl tributyl citrate via ingestion of food containing this compound, and dermal contact with consumer products (such as cosmetic, paints and inks) containing acetyl tributyl citrate. (SRC)

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

## 11.2.2 Natural Pollution Sources



Acetyl tributyl citrate is not reported as found in nature.

*Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed. Boca Raton, FL 2005, p. 1818*

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

## 11.2.3 Artificial Pollution Sources



Acetyl tributyl citrate's production and use as a plasticizer for vinyl and other resin(1,2), as a solvent and functional fluid in adhesives, paints, coating and inks(2) as a flavor ingredient(3) and in nail enamel(4) may result in its release to the environment through various waste streams(SRC).

(1) Lewis RJ Sr; *Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY, p. 15 (2007)* (2) US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2) (3) Burdock GA, ed; Fenaroli's Handbook of Flavor Ingredients. 5th ed. Boca Raton, FL: CRC Press, pp. 1817-1818 (2004) (4) National Library of Medicine Household Products Database. Available from, as of Jun 23, 2015: <http://hpd.nlm.nih.gov/>

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

## 11.2.4 Environmental Fate



TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 3280(SRC), determined from a log Kow of 4.90(2) and a regression-derived equation(3), indicates that acetyl tributyl citrate is expected to have slight mobility in soil(SRC). Volatilization of acetyl tributyl citrate from moist soil surfaces is expected to be an important fate process(SRC) given an estimated Henry's Law constant of  $3.2 \times 10^{-5}$  atm-cu m/mole(SRC), derived from its estimated vapor pressure,  $3 \times 10^{-4}$  mm Hg(3), and [water](#) solubility, 5 mg/L(4). However, adsorption to soil is expected to attenuate volatilization(SRC). Acetyl tributyl citrate is not expected to volatilize from dry soil surfaces(SRC) based upon its estimated vapor pressure of  $3 \times 10^{-4}$  mm Hg at 25 °C(SRC), determined from a fragment constant method(3). An 82% of theoretical BOD using activated sludge in the Japanese MITI test(5) suggests that biodegradation is an important environmental fate process in soil(SRC). Acetyl tributyl citrate was shown to biodegrade extensively in several other biodegradation studies and simulation tests(6,7). Two soil degradation studies observed rapid biomineralization of acetyl tributyl citrate(7).

(1) Swann RL et al; *Res Rev 85: 17-28 (1983)* (2) US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2) (3) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 15, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (4) Chemicals Inspection and Testing Institute; Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chem Indus Ecol- Toxicol Informat Center. ISBN 4-89074-101-1 (1992) (5) NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of June 15, 2015: <http://www.safe.nite.go.jp/english/db.html> (6) US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2) (7) US EPA; High Production Volume (HPV) Challenge Program. The HPV voluntary challenge chemical list. Robust summaries and test plans. Acetyl Tributyl Citrate. Washington, DC: US EPA, Off. Prevent. Pest. Tox. Subst., Pollut. Prevent. Toxics. Available from, as of June 16, 2015: <http://www.epa.gov/opptintr/chemrtk/>

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

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 3,280(SRC), determined from a log Kow of 4.92(2) and a regression-derived equation(3), indicates that acetyl tributyl citrate is expected to adsorb to suspended solids and sediment(SRC). Volatilization from [water](#) surfaces is expected(4) based upon an estimated Henry's Law constant of  $3.2 \times 10^{-5}$  atm-cu m/mole(SRC), derived from its estimated vapor pressure,  $3 \times 10^{-4}$  mm Hg(3), and [water](#) solubility, 5 mg/L(5). Using this Henry's Law constant and an estimation method(4), volatilization half-lives for a model river and model lake are 2.6 and 25 days, respectively(SRC). However, volatilization from [water](#) surfaces is expected to be attenuated by adsorption to suspended solids and sediment in the [water](#) column. The estimated volatilization half-life from a model pond is 335 days if adsorption is considered(6). According to a classification scheme(7), an estimated BCF of 35(SRC), from its log Kow and a regression-derived equation(3) suggests the potential for bioconcentration in aquatic organisms is moderate. An 82% of theoretical BOD using activated sludge in the Japanese MITI test(8) suggests that biodegradation is an important environmental fate process in [water](#)(SRC). Acetyl tributyl citrate was shown to biodegrade extensively in several other biodegradation studies and simulation tests(9,10). A base-catalyzed second-order hydrolysis rate constant of  $5.8 \times 10^{-2}$  L/mole-sec(SRC) was estimated using a structure estimation method(3); this corresponds to half-lives of 3.8 years and 140 days at pH values of 7 and 8, respectively(3). [



(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2) (3) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 15, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (5) Chemicals Inspection and Testing Institute; Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chem Indus Ecol- Toxicol Informat Center. ISBN 4-89074-101-1 (1992) (6) US EPA; EXAMS II Computer Simulation (1987) (7) Franke C et al; Chemosphere 29: 1501-14 (1994) (8) NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of June 15, 2015: <http://www.safe.nite.go.jp/english/db.html> (9) US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2) (10) US EPA; High Production Volume (HPV) Challenge Program. The HPV voluntary challenge chemical list. Robust summaries and test plans. Acetyl Tributyl Citrate. Washington, DC: US EPA, Off. Prevent. Pest. Tox. Subst., Pollut. Prevent. Toxics. Available from, as of June 16, 2015: <http://www.epa.gov/opptintr/chemrtk/>

▶ Hazardous Substances Data Bank (HSDB)

**ATMOSPHERIC FATE:** According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), acetyl tributyl citrate, which has an estimated vapor pressure of 3X10<sup>-4</sup> mm Hg at 25 °C(SRC), determined from a fragment constant method(2), is expected to exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase acetyl tributyl 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 27 hours(SRC), calculated from its rate constant of 1.4X10<sup>-11</sup> cu cm/molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(2). Particulate-phase acetyl tributyl citrate may be removed from the air by wet and dry deposition(SRC).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 15, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html>

▶ Hazardous Substances Data Bank (HSDB)

## 11.2.5 Environmental Biodegradation



**AEROBIC:** Acetyl tributyl citrate, present at an initial concentration of 30 mg/L, reached 82% of the theoretical BOD in 4 weeks with an activated sludge inoculum at 100 mg/L in the modified MITI test which classified the compound as readily biodegradable(1). Acetyl tributyl citrate was shown to biodegrade extensively in several other biodegradation studies and simulation tests(2,3). In a sewage column degradation test using acclimated sludge, acetyl tributyl citrate biodegraded >90% in hours(3). An aerobic biodegradation test in soil using a static biometer system found acetyl tributyl citrate to be readily biodegradable with theoretical CO<sub>2</sub> evolution of 72.9% to >100% (as various concentrations) over 42 days of incubation(3). A 52-day aerobic study in soil observed rapid biodegradation with mineralization (ThCO<sub>2</sub>) of 83 to >100% over 52 days(3).

(1) NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of June 15, 2015: <http://www.safe.nite.go.jp/english/db.html> (2) US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2) (3) US EPA; High Production Volume (HPV) Challenge Program. The HPV voluntary challenge chemical list. Robust summaries and test plans. Acetyl Tributyl Citrate. Washington, DC: US EPA, Off. Prevent. Pest. Tox. Subst., Pollut. Prevent. Toxics. Available from, as of June 16, 2015: <http://www.epa.gov/opptintr/chemrtk/>

▶ Hazardous Substances Data Bank (HSDB)

## 11.2.6 Environmental Abiotic Degradation



The rate constant for the vapor-phase reaction of acetyl tributyl citrate with photochemically-produced hydroxyl radicals has been estimated as 1.4X10<sup>-11</sup> cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 27 hours at an atmospheric concentration of 5X10<sup>+5</sup> hydroxyl radicals per cu cm(1). A base-catalyzed second-order hydrolysis rate constant of 5.8X10<sup>-2</sup> L/mole-sec(SRC) was estimated using a structure estimation method(1); this corresponds to half-lives of 3.8 years and 140 days at pH values of 7 and 8, respectively(1).

(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 15, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html>

▶ Hazardous Substances Data Bank (HSDB)

## 11.2.7 Environmental Bioconcentration



An estimated BCF of 35 was calculated in fish for acetyl tributyl citrate(SRC), using a log K<sub>ow</sub> of 4.92(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate(SRC), provided the compound is not metabolized by the organism(SRC).

(1) US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 15, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (3) Franke C et al; Chemosphere 29: 1501-14 (1994)

▶ Hazardous Substances Data Bank (HSDB)

## 11.2.8 Soil Adsorption/Mobility



The K<sub>oc</sub> of acetyl tributyl citrate is estimated as 3280(SRC), using a log K<sub>ow</sub> of 4.92(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated K<sub>oc</sub> value suggests that acetyl tributyl citrate is expected to have slight mobility in soil.

(1) US EPA; High Production Volume Information System (HPVIS). HPV Chemical Hazard Characterizations. Acetyl Tributyl Citrate (Casrn 77-90-7), September 2014. Available from, as of June 15, 2015: [http://iaspub.epa.gov/opthpv/hpv\\_hc\\_characterization.get\\_report?doctype=2](http://iaspub.epa.gov/opthpv/hpv_hc_characterization.get_report?doctype=2) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 15, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (3) Swann RL et al; Res Rev 85: 17-28 (1983)

▶ Hazardous Substances Data Bank (HSDB)

## 11.2.9 Volatilization from Water/Soil



The Henry's Law constant for acetyl tributyl citrate is estimated as  $3.2 \times 10^{-5}$  atm-cu m/mole(SRC) derived from its estimated vapor pressure,  $3.0 \times 10^{-4}$  mm Hg(1), and [water](#) solubility, 5 mg/L(2). This Henry's Law constant indicates that acetyl tributyl citrate is expected to volatilize from [water](#) surfaces(3). Based on this Henry's Law constant, the volatilization half-life from a model river (1 m deep, flowing 1 m/sec, wind velocity of 3 m/sec)(3) is estimated as 2.6 days(SRC). The volatilization half-life from a model lake (1 m deep, flowing 0.05 m/sec, wind velocity of 0.5 m/sec)(3) is estimated as 25 days(SRC). However, volatilization from [water](#) surfaces is expected to be attenuated by adsorption to suspended solids and sediment in the [water](#) column. The estimated volatilization half-life from a model pond is 335 days if adsorption is considered(4). Acetyl tributyl citrate's estimated Henry's Law constant indicates that volatilization from moist soil surfaces may occur, but the rate may be attenuated by adsorption to soil(SRC). Acetyl tributyl citrate is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(1).

(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of June 15, 2015: <http://www.epa.gov/oppt/exposure/pubs/episuite.html> (2) Chemicals Inspection and Testing Institute; Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chem Indus Ecol- Toxicol Informat Center. ISBN 4-89074-101-1 (1992) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (4) US EPA; EXAMS II Computer Simulation (1987)

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

## 11.2.10 Environmental Water Concentrations



**SURFACE WATER:** Acetyl tributyl citrate was identified in 2 [water](#) samples taken from the River Lee, Great Britain at trace levels(1).

(1) Waggott A; Chem Water Reuse 2: 55-9 (1981)

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

## 11.2.11 Food Survey Values



Acetyl tributyl citrate is reportedly used as a flavor ingredient in nonalcoholic beverages at a concentration of 1.0 ppm(1). A monitoring study of hospital diets in Japan for plasticizers in hospital food detected acetyl tributyl citrate at levels (in one hospital) that corresponded to a daily intake of 1228 ug/day(2); the source of the acetyl tributyl citrate in the food was suspected to be cling-film wrapping or other packaging(2). Monitoring tests determined that acetyl tributyl citrate plasticizer in plastic films migrated from the film into cooked poultry meat during microwave cooking(3).

(1) Burdock GA, ed; Fenaroli's Handbook of Flavor Ingredients. 5th ed. Boca Raton, FL: CRC Press, pp. 1817-1818 (2004) (2) Tsumura T et al; Food Addit Contam 20(4): 317-324 (2003) (3) Heath JL, Reilly M; Poult Sci 60(10): 2258-2264 (1981)

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

## 11.2.12 Other Environmental Concentrations



... Migration /citric acid, acetyl tributyl ester/ plasticizer from plasticized [polyvinylidene chloride-polyvinyl chloride](#) ...films into both olive oil and distilled [water](#) during microwave heating was studied. The amount of /citric acid, acetyl tributyl ester/ migrating into olive oil after heating for 10 min was 73.9 mg/L, into distilled [water](#) it was 4.1 mg/L after heating for 8 min.

Sheftel, V.O.; Indirect Food Additives and Polymers. Migration and Toxicology. Lewis Publishers, Boca Raton, FL. 2000, p. 193

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

Food-grade [polyvinyl chloride](#) (PVC) cling-film containing 5.3% (w/w) [di\(2-ethylhexyl\) adipate](#) (DEHA) and 3.0% (w/w) acetyltributyl citrate (ATBC) plasticizers was used to wrap halawa tehineh (halva) samples. Samples were split into two groups and stored at  $25 \pm 1$  degrees C. One group was analyzed for DEHA and ATBC content at intervals between 0.5 and 240hr of contact (kinetic study) and a second group was cut into slices (1.5mm thick) after 240hr of halva/PVC contact and was analyzed for DEHA and ATBC content (penetration study). Determination of both plasticizers was performed using a direct gas chromatographic (GC) method after extraction of DEHA from halva samples. DEHA readily migrated into halva samples: the equilibrium amount of DEHA in halva (3.31mg/sq dm film or 81.4mg/kg halva) corresponding to a loss of 54.7% (w/w) DEHA from PVC film. This value is slightly higher than the limit of 3mg/ sq dm of film surface set by the European Union for DEHA. The equilibrium amount of ATBC in halva was 1.46mg/sq dm (36.1mg/kg) corresponding to a loss of 42.7% ATBC from PVC film. With regard to the penetration of both plasticizers into halva samples, migration of DEHA was detectable up to the 7th slice beneath the surface of halva (total depth 10.5mm) while the migration of ATBC was detectable up to the 5th slice (total depth 7.5mm).

PMID:17141933

Goulas AE et al; Food Chem Toxicol. 45 (4): 585-91 (2007)

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

## 11.2.13 Probable Routes of Human Exposure



According to the 2012 TSCA Inventory Update Reporting data, 6 reporting facilities estimate the number of persons reasonably likely to be exposed in their respective industrial use in the United States manufacturing, processing, or use of acetyl tributyl citrate (77-90-7) may be as low as <10 workers up to the range of 50-99 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 15, 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 106,672 workers (98,182 of these are female) are potentially exposed to acetyl tributyl citrate in the US(1). Occupational exposure to acetyl tributyl citrate may occur through inhalation and dermal contact with this compound at workplaces where acetyl tributyl citrate is produced or used(SRC). Use data indicate that the general population may be exposed to acetyl tributyl citrate via inhalation of ambient air, ingestion of food containing this compound, and dermal contact with consumer products (such as cosmetics, paints and inks) containing acetyl tributyl 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). Available from, as of June 15, 2015: <http://www.cdc.gov/noes/>

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

## 12 Literature

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### 12.1 NLM Curated PubMed Citations

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▶ PubChem

### 12.2 Springer Nature References

---



▶ Springer Nature

### 12.3 Depositor Provided PubMed Citations

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▶ PubChem

## 12.4 Metabolite References

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

## 12.5 Chemical Co-Occurrences in Literature

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▶ [PubChem](#)

## 12.6 Chemical-Gene Co-Occurrences in Literature

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▶ [PubChem](#)

## 12.7 Chemical-Disease Co-Occurrences in Literature

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▶ [PubChem](#)

## 13 Patents



### 13.1 Depositor-Supplied Patent Identifiers



▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

### 13.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

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

▶ PATENTSCOPE (WIPO)

## 14 Biomolecular Interactions and Pathways

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### 14.1 Chemical-Gene Interactions

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#### 14.1.1 CTD Chemical-Gene Interactions

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▶ [Comparative Toxicogenomics Database \(CTD\)](#)



## 15 Biological Test Results

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### 15.1 BioAssay Results

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▶ PubChem

## 16 Classification

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### 16.1 Ontologies

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#### 16.1.1 MeSH Tree

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▶ Medical Subject Headings (MeSH)

#### 16.1.2 ChemIDplus

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▶ ChemIDplus

#### 16.1.3 UN GHS Classification

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

#### 16.1.4 EPA CPDat Classification

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- ▶ EPA Chemical and Products Database (CPDat)

#### 16.1.5 NORMAN Suspect List Exchange Classification

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- ▶ NORMAN Suspect List Exchange

#### 16.1.6 EPA DSSTox Classification

---



- ▶ EPA DSSTox

## 17 Information Sources



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## 1. ChemIDplus

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Acetyltributyl citrate [NF]

<https://chem.nlm.nih.gov/chemidplus/sid/0000077907>

ChemIDplus Chemical Information Classification

<https://chem.nlm.nih.gov/chemidplus/>

## 2. DTP/NCI

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Citroflex A

<https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=3894>

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1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, 1,2,3-tributyl ester

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## 4. EPA DSSTox

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Acetyl tributyl citrate

<https://comptox.epa.gov/dashboard/DTXSID2026446>

CompTox Chemicals Dashboard Chemical Lists

[https://comptox.epa.gov/dashboard/chemical\\_lists/](https://comptox.epa.gov/dashboard/chemical_lists/)

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<https://echa.europa.eu/substance-information/-/substanceinfo/100.000.971>

Tributyl O-acetylcitrate

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/111970>

## 6. Hazardous Substances Data Bank (HSDB)

ACETYL TRIBUTYL CITRATE

<https://pubchem.ncbi.nlm.nih.gov/source/hsdb/656>

## 7. Human Metabolome Database (HMDB)

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<http://www.hmdb.ca/citing>

Acetyl tributyl citrate

<http://www.hmdb.ca/metabolites/HMDB0034159>

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<http://ctdbase.org/about/legal.jsp><http://ctdbase.org/detail.go?type=chem&acc=C014953>

## 9. EPA Chemical and Products Database (CPDat)

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

tributyl acetyl citrate

<https://comptox.epa.gov/dashboard/DTXSID2026446#exposure>

EPA CPDat Classification

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

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

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*Tributyl acetylcitrate*

<http://www.fao.org/food/food-safety-quality/scientific-advice/jecfa/jecfa-flav/details/en/c/168/>

ACETYL TRIBUTYL CITRATE

<https://apps.who.int/food-additives-contaminants-jecfa-database/chemical.aspx?chemID=102>

11. [EU Food Improvement Agents](#)

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*NORMAN Suspect List Exchange Classification*

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

14. [FDA/SPL Indexing Data](#)

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*OZBX0N59RZ*

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

15. [Flavor and Extract Manufacturers Association \(FEMA\)](#)

*TRIBUTYL ACETYLCITRATE*

<https://www.femaflavor.org/flavor-library/tributyl-acetylcitrate>

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<https://foodb.ca/about>

*Acetyl tributyl citrate*

<https://foodb.ca/compounds/FDB012444>

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

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*2-ACETYLOXY-1,2,3-PROPANETRICARBOXYLIC ACID TRIBUTYL ESTER*

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

18. [NIST Mass Spectrometry Data Center](#)

*Tributyl acetylcitrate*

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

19. [SpectraBase](#)

*Acetyl tri-n-butyl citrate*

<https://spectrabase.com/spectrum/F30tEZtgV8j>

*Tributyl 2-acetylcitrate*

<https://spectrabase.com/spectrum/1MVZPzUIM7s>

*Tributyl O-acetylcitrate*

<https://spectrabase.com/spectrum/705mQoMTBgT>

*CITROFLEX A-4*

<https://spectrabase.com/spectrum/AJDxL3h4SEI>

*TRIBUTYL ACETYLCITRATE*

<https://spectrabase.com/spectrum/A5j5CZG1gT8>

*ACETYL TRI-n-BUTYL CITRATE*

<https://spectrabase.com/spectrum/KQU0qO4XOoe>

*CITRIC ACID, TRIBUTYL ESTER, ACETATE*

<https://spectrabase.com/spectrum/AGaLNHNz33k>

Tributyl 2-acetylcitrate

<https://spectrabase.com/spectrum/LDzgVG4WBN>

CITRIC ACID, TRIBUTYL ESTER, ACETATE

<https://spectrabase.com/spectrum/6Vjuc7g40m>

citric acid, tributyl ester, acetate

<https://spectrabase.com/spectrum/5LbuG2XHkeL>

CITRIC ACID, TRIBUTYL ESTER, ACETATE

<https://spectrabase.com/spectrum/KKVoHctOQW0>

Citric acid, tributyl ester acetate

<https://spectrabase.com/spectrum/Eajc5Tq8hxE>

CITRIC ACID, TRIBUTYL ESTER, ACETATE

<https://spectrabase.com/spectrum/C13guKzn91w>

Tributyl 2-acetylcitrate

<https://spectrabase.com/spectrum/8eSP10jTjHj>

Tributyl acetylcitrate

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

1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester

<https://spectrabase.com/spectrum/3umgPXs9oRM>

1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester

<https://spectrabase.com/spectrum/9NgL5up5J54>

1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester

<https://spectrabase.com/spectrum/Byn8HMDA7I8>

Acetyl tri-n-butyl citrate

<https://spectrabase.com/spectrum/3TTgQGk1npA>

1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester

<https://spectrabase.com/spectrum/7cJLuf9JwBM>

20. **Springer Nature**

<https://pubchem.ncbi.nlm.nih.gov/substance/341144566>

21. **Wikipedia**

acetyl tributyl citrate

<https://en.wikipedia.org/wiki/Acetyltributylcitrate>

22. **PubChem**

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

23. **MeSH**

2-acetyltributylcitrate

<https://www.ncbi.nlm.nih.gov/mesh/67014953>

24. **Medical Subject Headings (MeSH)**

MeSH Tree

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

25. **UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)**

GHS Classification Tree

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26. **PATENTSCOPE (WIPO)**

SID 403390809

<https://pubchem.ncbi.nlm.nih.gov/substance/403390809>