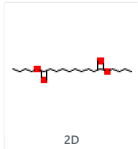



**COVID-19 is an emerging, rapidly evolving situation.**Get the latest public health information from CDC: <https://www.coronavirus.gov>.Get the latest research from NIH: <https://www.nih.gov/coronavirus>.

COMPOUND SUMMARY

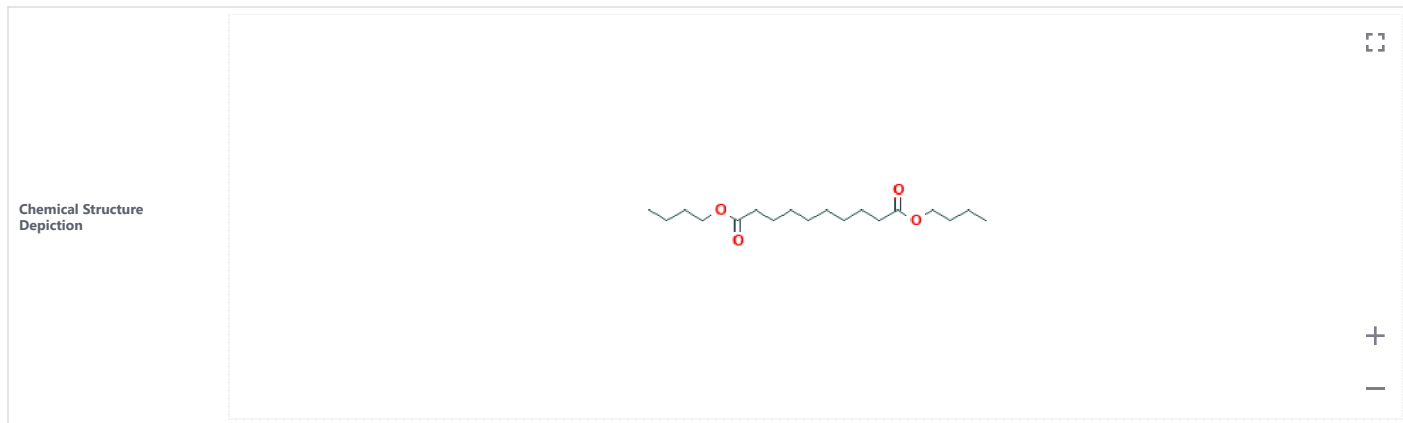
Dibutyl sebacate

PubChem CID	7986
Structure	 2D Find Similar Structures
Chemical Safety	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{18}H_{34}O_4$ or $CH_3(CH_2)_3O_2C(CH_2)_8CO_2(CH_2)_3CH_3$
Synonyms	DIBUTYL SEBACATE Dibutyl decanedioate 109-43-3 Butyl sebacate Di-n-butyl sebacate <input type="button" value="More..."/>
Molecular Weight	314.5 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

dibutyl decanedioate

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

[▶ PubChem](#)

2.1.2 InChI

InChI=1S/C18H34O4/c1-3-5-15-21-17(19)13-11-9-7-8-10-12-14-18(20)22-16-6-4-2/h3-16H2,1-2H3

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

[▶ PubChem](#)

2.1.3 InChI Key

PYGXAGIECVWIOZ-UHFFFAOYSA-N

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

[▶ PubChem](#)

2.1.4 Canonical SMILES

CCCCOC(=O)CCCCCCCCC(=O)OCCCC

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

[▶ PubChem](#)

2.2 Molecular Formula

C18H34O4

CH3(CH2)3O2C(CH2)8CO2(CH2)3CH3

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

C18H34O4

Computed by PubChem 2.1 (PubChem release 2019.06.18)

[▶ PubChem](#)

2.3 Other Identifiers

2.3.1 CAS

109-43-3

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

2.3.2 Deprecated CAS

39393-66-3, 98781-27-2

[▶ ChemIDplus](#)

2.3.3 European Community (EC) Number

203-672-5

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

2.3.4 ICSC Number

1349

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

2.3.5 NSC Number

3893

[▶ DTP/NCI](#)

2.3.6 RTECS Number



VS150000

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

2.3.7 UNII



4W5IH7FLNY

[▶ FDA/SPL Indexing Data](#)

2.3.8 JECFA Number



625

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

2.3.9 FEMA Number



2373

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

2.3.10 DSSTox Substance ID



DTXSID1041847

[▶ EPA DSSTox](#)

2.3.11 Wikipedia



Dibutyl sebacate

[▶ Wikipedia](#)

2.4 Synonyms



2.4.1 MeSH Entry Terms

dibutyl sebacate
dibutylsebacate[▶ MeSH](#)

2.4.2 Depositor-Supplied Synonyms



DIBUTYL SEBACATE	Sebacic acid, dibutyl ester	Sebacic acid dibutyl ester	BRN 1798308	ACMC-1BUY3	NSC3893
Dibutyl decanedioate	Di-n-butylsebacate	Uniflex DBS	A13-00393	EC 203-672-5	Dibutyl decanedioate 109-43-
109-43-3	Bis(n-butyl)sebacate	NSC 3893	MFC00027218	Dibutyl sebacate, >=90%	KS-00000YU3
Butyl sebacate	1,10-dibutyl decanedioate	Reomol DBS	Dibutyl sebacate, 93%	SCHEMBL42655	NSC-3893
Di-n-butyl sebacate	Dibutylester kyseliny sebakove	Decanedioic acid, 1,10-dibutyl ester	DSSTox_CID_21847	4-02-00-02081 (Beilstein Handbook Reference)	ZINC3875764
Decanedioic acid, dibutyl ester	Di(n-butyl) sebacate	FEMA No. 2373	DSSTox_RID_79856	KSC175Q6R	Tox21_113651
Polycizer DBS	PX 404	HSDB 309	DSSTox_GSID_41847	CHEMBL2106225	Tox21_300154
Kodaflex DBS	Decanedioic Acid Dibutyl Ester	Dibutyl sebacate (NF)	CAS-109-43-3	DTXSID1041847	ANW-16045
Dibutyl sebacinate	Dibutyl 1,8-octanedicarboxylate	Dibutyl sebacate [NF]	Di-n-butyl-sebacate	CTK0H5868	Dibutyl sebacate, analytical st
Staffex DBS	UNII-4W5IH7FLNY	EINECS 203-672-5	Di-n-butyl decanedioate	FEMA 2373	LMFA07010828
Monoplex DBS	n-Butyl sebacate	4W5IH7FLNY	CCRIS 8264	Sebacic acid, bis-n-butyl ester	s6041
Bis(n-butyl) sebacate	Plasthall DBS	Dibutylester kyseliny sebakove [Czech]	di-butyl sebacate	Dibutyl sebacate, technical grade	Dibutyl sebacate, >=97.0% (G

[▶ PubChem](#)

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	314.5 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
XLogP3-AA	5.3	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	4	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	17	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	314.24571 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Monoisotopic Mass	314.24571 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Topological Polar Surface Area	52.6 Å ²	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	22	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	248	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2019.01.04)

► PubChem

3.2 Experimental Properties



3.2.1 Physical Description



Liquid

► EPA Chemicals under the TSCA; Human Metabolome Database (HMDB)

COLOURLESS OILY LIQUID.

► ILO International Chemical Safety Cards (ICSC)

colourless to oily liquid; fruity but very mild odour with a very faint fruity oily taste

► Joint FAO/WHO Expert Committee on Food Additives (JECFA)

3.2.2 Color/Form



Colorless liquid

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 359

► Hazardous Substances Data Bank (HSDB)

3.2.3 Odor



Odorless

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 359

► Hazardous Substances Data Bank (HSDB)

3.2.4 Boiling Point



344.5 °C

► EPA DSSTox; Hazardous Substances Data Bank (HSDB)

344-345 °C

► ILO International Chemical Safety Cards (ICSC)

3.2.5 Melting Point



-10.0 °C

► EPA DSSTox

-10 °C

Lide, D.R. (ed.). *CRC Handbook of Chemistry and Physics*. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999, p. 3-140

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

12°C

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

3.2.6 Flash Point



353 °F (178 °C) (OPEN CUP)

Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-33

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

167 °C

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

3.2.7 Solubility



1.27e-04 M

RIDDICK,JA ET AL. (1986)

▶ [EPA DSSTox](#)

Soluble in ethyl ether

Lide, D.R. (ed.). *CRC Handbook of Chemistry and Physics*. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999, p. 3-140

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

water solubility = 40 mg/l @ 20 °C

Riddick, J.A., W.B. Bunger, Sakano T.K. *Techniques of Chemistry 4th ed., Volume II. Organic Solvents*. New York, NY: John Wiley and Sons, 1985.

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

0.04 mg/mL at 20 °C

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

Solubility in water: none

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

insoluble in water; soluble in alcohol; miscible in oil

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

3.2.8 Density



0.9405 @ 15 °C

Lide, D.R. (ed.). *CRC Handbook of Chemistry and Physics*. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999, p. 3-140

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

Relative density (water = 1): 0.9

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

0.936-0.940 (20Å°)

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

3.2.9 Vapor Density



10.8 (Air= 1)

Sax, N.I. *Dangerous Properties of Industrial Materials*. Vol 1-3 7th ed. New York, NY: Van Nostrand Reinhold, 1989, p. 1126

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

Relative vapor density (air = 1): 10.8

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

3.2.10 Vapor Pressure



4.69e-06 mmHg

▶ [EPA DSSTox](#)

4.69X10⁻⁶ mm Hg @ 25 °C

Daubert, T.E., R.P. Danner. *Physical and Thermodynamic Properties of Pure Chemicals Data Compilation*. Washington, D.C.: Taylor and Francis, 1989.

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

3.2.11 Autoignition Temperature



690 °F (365 °C)

Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-33

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

3.2.12 Decomposition



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

Lewis, R.J. *Sax's Dangerous Properties of Industrial Materials*. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1081

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

3.2.13 Refractive Index



Index of refraction: 1.4433 @ 15 °C/D

Lide, D.R. (ed.). *CRC Handbook of Chemistry and Physics*. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999., p. 3-140

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

1.439-1.444

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

3.2.14 Kovats Retention Index



Standard non-polar	2137, 2140, 2169, 2137, 2137
Semi-standard non-polar	2180.1, 2138.7

► [NIST Mass Spectrometry Data Center](#)

4 Spectral Information



4.1 1D NMR Spectra



1D NMR Spectra NMR: 7636 (Sadtler Research Laboratories Spectral Collection)

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

1D NMR Spectra [1D NMR Spectrum 2131 - Dibutyl decanedioate \(HMDB0041220\)](#)

[1D NMR Spectrum 2818 - Dibutyl decanedioate \(HMDB0041220\)](#)

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

4.1.1 1H NMR Spectra



Instrument Name Varian A-60

Source of Sample Wallace & Tiernan, Inc., Belleville, New Jersey

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Thumbnail

▶ [SpectraBase](#)

4.1.2 13C NMR Spectra



Source of Sample Wallace & Tiernan, Inc., Belleville, New Jersey

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Thumbnail

▶ [SpectraBase](#)

Instrument Name Varian HA-100

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Thumbnail

[▶ SpectraBase](#)

4.2 Mass Spectrometry



Showing 2 of 9 [View More](#)

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

[▶ SpectraBase](#)

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](#)

4.2.1 GC-MS



Showing 2 of 9 [View More](#)

GC-MS	GC-MS Spectrum 27121 - Dibutyl decanedioate (HMDB0041220) GC-MS Spectrum 27122 - Dibutyl decanedioate (HMDB0041220) GC-MS Spectrum 102196 - Dibutyl decanedioate (HMDB0041220) GC-MS Spectrum 102197 - Dibutyl decanedioate (HMDB0041220)
-------	--

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

MoNA ID	JP001710
MS Category	Experimental
MS Type	GC-MS
MS Level	MS1
Instrument	Unknown
Instrument Type	El-B
Ionization Mode	positive
Splash	splash10-052p-791000000-ddef7e520d4682270616
Thumbnail	

Submitter University of Tokyo Team, Faculty of Engineering, University of Tokyo

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

4.2.2 MS-MS



NIST Number	1118498
Instrument Type	IT/ion trap
Collision Energy	0
Spectrum Type	MS2
Precursor Type	[M+H] ⁺
Precursor m/z	315.253
Total Peaks	10
m/z Top Peak	241.2
m/z 2nd Highest	185.2
m/z 3rd Highest	258.9

Thumbnail

► [NIST Mass Spectrometry Data Center](#)

4.2.3 EI-MS



EI-MS [EI-MS Spectrum 461 - Dibutyl decanedioate \(HMDB0041220\)](#)

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

4.2.4 Other MS



Other MS [MASS: 1929 \(Atlas of Mass Spectral Data, John Wiley & Sons, New York\)](#)

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

4.3 IR Spectra



IR Spectra [IR: 15101 \(Sadtler Research Laboratories IR Grating Collection\)](#)

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

4.3.1 FTIR Spectra



Showing 2 of 8 [View More](#)

Technique	BETWEEN SALTS
Source of Sample	Wallace & Tiernan, Inc., Harchem Division

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Thumbnail

▶ SpectraBase

Technique CAPILLARY CELL: NEAT

Source of Sample Wallace & Tiernan, Inc., Belleville, New Jersey

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Thumbnail

▶ SpectraBase

4.3.2 ATR-IR Spectra



Showing 2 of 3 [View More](#)

Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DurasampIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	Scientific Polymer Products, Inc.
Catalog Number	P-173
Lot Number	591227002
Copyright	Copyright © 2012-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

▶ SpectraBase

Technique ATR-Neat

Copyright © 1980, 1981-2020 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

► SpectraBase

4.3.3 Near IR Spectra



Technique	NIR Path Length= 0.5/20 Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=12006,REO=2,CNM=HEI,ZFF=2 Spectrometer= BRUKER IFS 88
Source of Spectrum	Prof. Buback, University of Goettingen, Germany
Copyright	Copyright © 1989, 1990-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

► SpectraBase

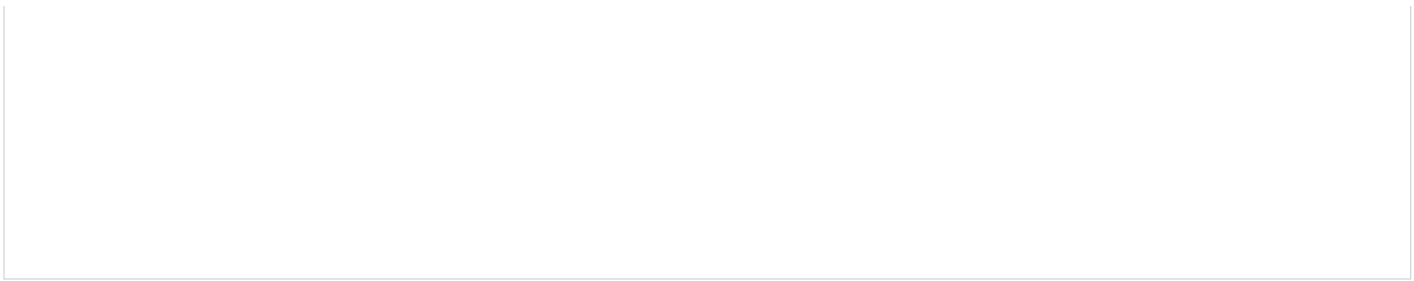
Technique	NIR Path Length= 0.5/20 Spectrometer= INSTRUMENT PARAMETERS=INST=BRUKER,RSN=12006,REO=2,CNM=HEI,ZFF=2 Spectrometer= BRUKER IFS 88
Source of Spectrum	Prof. Buback, University of Goettingen, Germany
Copyright	Copyright © 1989, 1990-2020 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.
Thumbnail	

► SpectraBase

4.3.4 Vapor Phase IR Spectra



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



▶ [SpectraBase](#)

4.4 Other Spectra



SADTLER REFERENCE NUMBER: 983 (IR, PRISM)

Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-271

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

5 Related Records



5.1 Related Compounds with Annotation



▶ PubChem

5.2 Related Compounds



Same Parent, Exact	10 Records
Mixtures, Components, and Neutralized Forms	43 Records
Similar Compounds	4,667 Records

▶ PubChem

5.3 Substances



5.3.1 Related Substances



All	166 Records
Same	121 Records
Mixture	45 Records

▶ PubChem

5.3.2 Substances by Category



▶ PubChem

5.4 Entrez Crosslinks



PubMed	57 Records
--------	------------

▶ PubChem

6 Chemical Vendors



▶ 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



Fruit

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

7.3 FDA Substances Added to Food



Substance	DIBUTYL SEBACATE
Used for (Technical Effect)	FLAVORING AGENT OR ADJUVANT
Document Number (21 CFR)	172.515 175.105 175.300 175.320 176.170 177.2600 178.3910 181.27

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

7.4 Organoleptic Properties



Flavors

oily
faint
fruity

- ▶ [FooDB](#)

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



Chemical Name	BUTYL SEBACATE
Evaluation Year	2002
ADI	No safety concern at current levels of intake when used as a flavouring agent
Comments	Secondary components do not raise a safety concern
Report	TRS 913-JECFA 59/111

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

8 Pharmacology and Biochemistry



8.1 Metabolism/Metabolites



IN VITRO PANCREATIC LIPASE HYDROLYZES DIBUTYL SEBACATE AS RAPIDLY AS IT DOES **TRIOLEIN**, & FROM THIS IT CAN BE CONCLUDED THAT THE PLASTICIZER IS METABOLIZED IN THE BODY BY SAME ROUTE AS FATS.

Lefaux, R. Practical Toxicology of Plastics. Cleveland: CRC Press Inc., 1968., p. 363

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

8.2 Human Metabolite Information



8.2.1 Cellular Locations



Extracellular
Membrane

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

9 Use and Manufacturing




9.1 Use Classification



EPA Safer Chemical Functional Use Classes -> Emollients;Skin Conditioning Agents;Solvents

▶ EPA Safer Choice

Safer Chemical Classes ->  Green circle - The chemical has been verified to be of low concern

▶ EPA Safer Choice

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 -> Emollient; Film forming; Hair conditioning; Plasticiser; Skin conditioning

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

▶ NORMAN Suspect List Exchange

9.2 Uses



EPA CPDat Chemical and Product Categories

▶ EPA Chemical and Products Database (CPDat)

SYNTHETIC FLAVORING ADJUVANT

Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 125

▶ Hazardous Substances Data Bank (HSDB)

Plasticizer, rubber softener, dielectric liquid, cosmetic and perfumes, flavoring ingredient

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 359

▶ Hazardous Substances Data Bank (HSDB)

9.2.1 Industry Uses



Pigments
Plasticizers
Solvents (which become part of product formulation or mixture)

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

▶ EPA Chemicals under the TSCA

9.2.2 Consumer Uses



Ink, toner, and colorant products
Photographic supplies, film, and photo chemicals

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

▶ EPA Chemicals under the TSCA

9.3 Methods of Manufacturing



BY DISTILLATION OF **SEBACIC ACID** WITH **BUTYL ALCOHOL** IN PRESENCE OF CONC N HCL IN **BENZENE** SOLN OR BY REACTING **BUTYL ALCOHOL** & **SEBACYL CHLORIDE**...

Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 125

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

9.4 U.S. Production



Aggregated Product Volume (EPA CDR 2016)

500,000 - 1,000,000 lb

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

▶ [EPA Chemicals under the TSCA](#)

(1972) 2.04X10+9 GRAMS

SRI

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

(1975) 2.54X10+9 G (INCL 2-ETHYLHEXYL)

SRI

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

9.5 General Manufacturing Information



Industry Processing Sectors

Pharmaceutical and medicine manufacturing
Photographic film paper, plate, and chemical manufacturing
Plastic material and resin manufacturing
Plastics product manufacturing
Printing ink manufacturing
Rubber product manufacturing
Synthetic rubber manufacturing
Wholesale and retail trade

▶ [EPA Chemicals under the TSCA](#)

EPA TSCA Commercial Activity Status

Decanedioic acid, 1,10-dibutyl ester: ACTIVE

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

▶ [EPA Chemicals under the TSCA](#)

REPORTED USES: NON-ALCOHOLIC BEVERAGES 1.0-5.0; **ICE CREAM**, ICES, ETC 2.0-5.0 PPM; CANDY 15 PPM; BAKED GOODS 15 PPM.

Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 125

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

DIBUTYL SEBACATE IS A VERY GOOD PLASTICIZER FOR **POLYVINYL CHLORIDE**, TO WHICH IT IMPARTS EXCELLENT LOW-TEMPERATURE RESISTANCE, FLEXIBILITY BEING RETAINED OVER WIDE TEMP RANGE.

Lefaux, R. Practical Toxicology of Plastics. Cleveland: CRC Press Inc., 1968., p. 362

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

IT IS...PLASTICIZER OF CHOICE FOR **CELLULOSE** ACETOBUTYRATE, POLYVINYL BUTYRAL, RUBBER HYDROCHLORIDE, & **POLYVINYLIDENE CHLORIDE**. IT IS EQUALLY COMPATIBLE WITH **NITROCELLULOSE**, **ETHYL CELLULOSE**, POLYSTYRENE, & MANY SYNTHETIC RUBBERS.

Lefaux, R. Practical Toxicology of Plastics. Cleveland: CRC Press Inc., 1968., p. 362

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

...ITS USE IN FOOD-PACKAGING INDUSTRY IS AUTHORIZED IN FRANCE, US, & ITALY.

Lefaux, R. Practical Toxicology of Plastics. Cleveland: CRC Press Inc., 1968., p. 363

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

10 Identification



10.1 Analytic Laboratory Methods



DIBUTYL SEBACATE, ADDITIVE IN PVDC FILM, WAS EXTRACTED BY SOLVENTS IN FATTY FOODS & DETERMINED BY GAS CHROMATOGRAPHY.

MOTEGI S ET AL; STUDIES OF MIGRATION OF ADDITIVES FROM POLYVINYLIDENE CHLORIDE FILM INTO FATTY FOODS; BULL JPN SOC SCI FISH 44(7) 789-796 (1978)

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

GAS-CHROMATOGRAPHIC DETERMINATION OF DIBUTYL SEBACATE IN AIR OF INDUSTRIAL PREMISES.

PERTSOVSKII AL, MARKOVSKAYA TV; GAS-CHROMATOGRAPHIC DETERMINATION OF DIBUTYL SEBACATE IN AIR OF INDUSTRIAL PREMISES; AKTUAL VOPR OKHR TR KHIM PROM-STI 93-4 (1976)

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

11 Safety and Hazards




11.1 Hazards Identification



11.1.1 GHS Classification



Pictogram(s)	 Irritant
Signal	Warning
GHS Hazard Statements	H315 (98.56%): Causes skin irritation [Warning Skin corrosion/irritation] H319 (98.56%): Causes serious eye irritation [Warning Serious eye damage/eye irritation] H335 (97.84%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]
Precautionary Statement Codes	P261, P264, P271, P280, P302+P352, P304+P340, P305+P351+P338, P312, P321, P332+P313, P337+P313, P362, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	<i>Aggregated GHS information provided by 463 companies from 12 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies. Reported as not meeting GHS hazard criteria by 324 of 463 companies. For more detailed information, please visit ECHA C&L website. Of the 10 notification(s) provided by 139 of 463 companies with hazard statement code(s). Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.</i>

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

11.1.2 Hazard Classes and Categories



Skin Irrit. 2 (98.56%)


Eye Irrit. 2 (98.56%)

STOT SE 3 (97.84%)

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

11.1.3 NFPA Hazard Classification



NFPA 704 Diamond	 0-1-0
NFPA Health Rating	0 - Materials that, under emergency conditions, would offer no hazard beyond that of ordinary combustible materials.
NFPA Fire Rating	1 - Materials that must be preheated before ignition can occur. Materials require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur.
NFPA Instability Rating	0 - Materials that in themselves are normally stable, even under fire conditions.

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

11.1.4 EPA Safer Chemical



Chemical: Dibutyl sebacate



Green circle - The chemical has been verified to be of low concern based on experimental and modeled data.

► [EPA Safer Choice](#)

11.1.5 Fire Hazards



Combustible.

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

11.2 First Aid Measures



11.2.1 Inhalation First Aid



Fresh air, rest.

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

11.2.2 Skin First Aid



Remove contaminated clothes. Rinse and then wash skin with **water** and soap.

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

11.2.3 Eye First Aid



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

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

11.2.4 Ingestion First Aid



Rinse mouth. Rest.

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

11.3 Fire Fighting



Use [water](#) spray, powder, [carbon dioxide](#).

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

11.3.1 Fire Fighting Procedures



...[CARBON DIOXIDE](#), DRY CHEM.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1081

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

11.4 Accidental Release Measures



11.4.1 Spillage Disposal



Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Carefully collect remainder. Then store and dispose of according to local regulations.

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

11.4.2 Disposal Methods



SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

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

11.5 Handling and Storage



11.5.1 Safe Storage



Well closed.

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

11.6 Exposure Control and Personal Protection



11.6.1 Inhalation Risk



A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20 °C; on spraying or dispersing, however, much faster.

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

11.6.2 Effects of Long Term Exposure



Repeated or prolonged contact may cause skin sensitization.

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

11.6.3 Fire Prevention



NO open flames.

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

11.6.4 Exposure Prevention



STRICT HYGIENE!

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

11.6.5 Inhalation Prevention



Use ventilation.

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

11.6.6 Skin Prevention



Protective gloves. Protective clothing.

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

11.6.7 Eye Prevention



Wear safety goggles.

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

11.6.8 Ingestion Prevention



Do not eat, drink, or smoke during work.

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

11.7 Stability and Reactivity



11.7.1 Hazardous Reactivities and Incompatibilities



Combustible liquid when exposed to heat or flame; can react with oxidizing materials.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1081

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

11.8 Regulatory Information



11.8.1 FDA Requirements



Dibutyl sebacate is a 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 2) 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.

21 CFR 172.515 (4/1/99)

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

Dibutyl sebacate is an indirect food additive for use only as a component of adhesives.

21 CFR 175.105 (4/1/99)

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

Prior-Sanctioned Food Ingredients: Substances classified as plasticizers, when migrating from food-packaging material shall include: dibutyl sebacate.

21 CFR 181.27 (4/1/99)

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

12 Toxicity



12.1 Toxicological Information



12.1.1 NIOSH Toxicity Data



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

12.1.2 Acute Effects



► [ChemIDplus](#)

12.1.3 Non-Human Toxicity Excerpts



...In a 2 yr period study, dietary levels of 0.25, 1.25, and 6.25% dibutyl sebacate were fed to rats. The data showed no weight, hematologic, or bone marrow changes, but some isolated inflammatory changes in the lungs, some nephrosis and fatty livers at the highest dose.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3042

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

Toxicologic data indicate that the material is practically nontoxic orally or by dermal contact.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3036

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

ORAL /ACUTE/ TOXICITY. DOSES OF 1-32 G/KG BODY WT WERE ADMIN TO YOUNG RATS 5-10 WK OLD & WEIGHING 60-75 G. ALL DOSES UP TO 16 G/KG WERE TOLERATED... DOSES OF 4-8 G/KG BODY WT WERE ADMIN TO RATS IM WITHOUT PRODUCING ANY OBSERVABLE REACTIONS.

Lefaux, R. Practical Toxicology of Plastics. Cleveland: CRC Press Inc., 1968., p. 362

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

12.1.4 Human Toxicity Values



Mildly toxic by ingestion. Experimental reproductive effects.

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1081

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

12.1.5 Non-Human Toxicity Values



LD50 Rat oral 16-32 g/kg

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3036

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

LD50 Rat oral 16.0 g/kg

Clayton, G.D., F.E. Clayton (eds.) *Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F. Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3036*

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

LD50 Rat oral 16 g/kg

Lewis, R.J. *Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 1081*

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

12.2 Ecological Information



12.2.1 Environmental Fate/Exposure Summary



Dibutyl sebacate's production and use as a plasticizer, rubber softener, flavoring agent and cosmetic and perfume additive may result in its release to the environment through its use and from various waste streams. If released to air, a vapor pressure of 4.7X10⁻⁶ mm Hg at 25 °C indicates dibutyl sebacate will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase dibutyl sebacate 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 21 hours. Particulate-phase dibutyl sebacate will be removed from the atmosphere by wet and dry deposition. Dibutyl sebacate may also undergo direct photolysis since it contains a functional group that can absorb light greater than 290 nm, but the kinetics of this reaction are unknown. If released to soil, dibutyl sebacate is expected to have low mobility based upon an estimated K_{oc} of 575. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 4.8X10⁻⁸ atm-cu m/mole. Volatilization from dry soil surfaces is not expected to be an important fate process based upon the vapor pressure. Dibutyl sebacate and other plasticizers were readily biodegraded by pure cultures. If released into [water](#), dibutyl sebacate is expected to adsorb to suspended solids and sediment in [water](#) based upon the estimated K_{oc}. Volatilization from [water](#) surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. Hydrolysis is expected to occur slowly in the environment based on estimated hydrolysis half-lives of 166 days and 4.5 years at pH 8 and 7, respectively. An estimated BCF of 77 suggests the potential for bioconcentration in aquatic organisms is moderate. Occupational exposure to dibutyl sebacate may occur through inhalation and dermal contact with this compound at workplaces where dibutyl sebacate is produced or used. The general population is exposed to dibutyl sebacate through the use of consumer products that contain this compound. (SRC)

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

12.2.2 Natural Pollution Sources



NOT REPORTED FOUND IN NATURE.

Fenaroli's *Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 125*

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

12.2.3 Artificial Pollution Sources



Dibutyl sebacate's production and use as a plasticizer, rubber softener, flavoring agent and cosmetic and perfume ingredient(1) may result in its release to the environment through various waste streams(SRC).

(1) Lewis RJ; *Hawley's Condensed Chemical Dictionary. 13th ed. NY, NY: Van Nostrand Reinhold Co pp. 359 (1997)*

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

12.2.4 Environmental Fate



TERRESTRIAL FATE: Based on a classification scheme(1), an estimated K_{oc} value of 575(SRC), determined from a [water](#) solubility of 40 mg/l(2) and a regression-derived equation(3), indicates that dibutyl sebacate is expected to have low mobility in soil(SRC). Volatilization of dibutyl sebacate from moist soil surfaces is not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 4.8X10⁻⁸ atm-cu m/mole(SRC), calculated from a vapor pressure of 4.7X10⁻⁶ mm Hg(4) and [water](#) solubility of 40 mg/l(2). Dibutyl sebacate is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(4). Dibutyl sebacate and other plasticizers were readily biodegraded by pure bacterial and fungal cultures(5,6).

(1) Swann RL et al; *Res Rev 85: 17-28 (1983)* (2) Riddick JA et al; *Organic Solvents: Physical Properties and Methods of Purification 4th ed NY, NY: Wiley Interscience (1986)* (3) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-5 (1990)* (4) Daubert TE, Danner RP; *Physical and Thermodynamic Properties of Pure Chemicals Data Compilation Washington, DC: Taylor and Francis (1996)* (5) Osmon JL et al; pp. 66-75 in *Proc Int Biodeterior Symp. 2nd (1972)* (6) Klausmeier RE, Jones WA; *Dev Ind Microbiol 2: 47-53 (1960)*

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

AQUATIC FATE: Based on a classification scheme(1), an estimated K_{oc} value of 575(SRC), determined from a [water](#) solubility of 40 mg/l(2) and a regression-derived equation(3), indicates that dibutyl sebacate is expected to adsorb to suspended solids and sediment in [water](#)(SRC). Volatilization from [water](#) surfaces is not expected to be an important fate process(3) based upon an estimated Henry's Law constant of 4.8X10⁻⁸ atm-cu m/mole(SRC), calculated from a vapor pressure of 4.7X10⁻⁶ mm Hg(4) and [water](#) solubility of 40 mg/l(2). A base-catalyzed second-order hydrolysis rate constant of 0.05 L/mole-sec(SRC) was estimated using a structure estimation method(5); this corresponds to half-lives of 4.5 years and 166 days at pH values of 7 and 8, respectively(5). Dibutyl sebacate and other plasticizers were readily biodegraded by pure bacterial and fungal cultures(6,7). According to a classification scheme(8), an estimated BCF of 77(SRC), from its [water](#) solubility(2) and a regression-derived equation(3), suggests the potential for bioconcentration in aquatic organisms is moderate(SRC).

(1) Swann RL et al; *Res Rev 85: 17-28 (1983)* (2) Riddick JA et al; *Organic Solvents: Physical Properties and Methods of Purification 4th ed Wiley Interscience NY (1986)* (3) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-5, 5-3, 15-1 to 15-29 (1990)* (4) Daubert TE, Danner RP; *Physical and Thermodynamic Properties of Pure Chemicals Data Compilation Washington, DC: Taylor and Francis (1996)* (5) Mill T et al; *Environmental Fate and Exposure Studies Development of a PC-SAR for Hydrolysis: Esters, Alkyl Halides and Epoxides. EPA Contract No. 68-02-4254. Menlo Park, CA: SRI International (1987)* (6) Osmon JL et al; pp. 66-75 in *Proc Int Biodeterior Symp. 2nd (1972)* (7) Klausmeier RE, Jones WA; *Dev Ind Microbiol 2: 47-53 (1960)* (8) Franke C et al; *Chemosphere 29: 1501-14 (1994)*

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

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), dibutyl sebacate, which has a vapor pressure of 4.7X10⁻⁶ mm Hg at 25 °C(2), is expected to exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase dibutyl sebacate 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 21 hours(SRC), calculated from its estimated rate constant of 1.8X10⁻¹¹ cu cm/molecule-sec at 25 °C(SRC) determined using a structure estimation method(3). Particulate-phase dibutyl sebacate may be removed from the air by wet and dry deposition(SRC). Dibutyl sebacate may also undergo direct photolysis in the environment since this compound contains functional groups that can absorb light greater than 290 nm(4).

(1) Bidleman TF; *Environ Sci Technol 22: 361-367 (1988)* (2) Daubert TE, Danner RP; *Physical and Thermodynamic Properties of Pure Chemicals Data Compilation Washington, DC: Taylor and Francis (1996)* (3) Meylan WM, Howard PH; *Chemosphere 26: 2293-99 (1993)* (4) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-13 (1990)*

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

12.2.5 Environmental Biodegradation



Dibutyl sebacate was degraded by pure bacterial and fungal cultures over 1 to 4 week incubation periods in shake flask experiments(1). Pure strains of the fungus *Fusarium* were shown to degrade dibutyl sebacate and several other plasticizers(2).

(1) Osmon JL et al; pp. 66-75 in *Proc Int Biodeterior Symp. 2nd (1972)* (2) Klausmeier RE, Jones WA; *Dev Ind Microbiol* 2: 47-53 (1960)

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

12.2.6 Environmental Abiotic Degradation



The rate constant for the vapor-phase reaction of dibutyl sebacate with photochemically-produced hydroxyl radicals has been estimated as 1.8×10^{-11} cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 21 hours at an atmospheric concentration of 5×10^5 hydroxyl radicals per cu cm(1). A base-catalyzed second-order hydrolysis rate constant of 0.05 L/mole-sec(SRC) was estimated using a structure estimation method(2); this corresponds to half-lives of 4.5 years and 166 days at pH values of 7 and 8, respectively(2). The expected hydrolysis products are [butanol](#) and [sebacic acid](#). Dibutyl sebacate may also undergo direct photolysis in the environment since this compound contain a functional group that can absorb light greater than 290 nm(3).

(1) Meylan WM, Howard PH; *Chemosphere* 26: 2293-99 (1993) (2) Mill T et al; *Environmental Fate and Exposure Studies Development of a PC-SAR for Hydrolysis: Esters, Alkyl Halides and Epoxides. EPA Contract No. 68-02-4254. Menlo Park, CA: SRI International (1987)* (3) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-13 (1990)*

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

12.2.7 Environmental Bioconcentration



An estimated BCF of 77 was calculated for dibutyl sebacate(SRC), using a [water](#) solubility of 40 mg/l(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Riddick JA et al; *Organic Solvents: Physical Properties and Methods of Purification 4th ed NY, NY: Wiley Interscience (1986)* (2) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 5-3 (1990)* (3) Franke C et al; *Chemosphere* 29: 1501-14 (1994)

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

12.2.8 Soil Adsorption/Mobility



The Koc of dibutyl sebacate is estimated as 575(SRC), using a [water](#) solubility of 40 mg/l(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that dibutyl sebacate is expected to have low mobility in soil(SRC).

(1) Riddick JA et al; *Organic Solvents: Physical Properties and Methods of Purification. 4th ed NY, NY: Wiley Interscience (1986)* (2) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-5 (1990)* (3) Swann RL et al; *Res Rev* 85: 17-28 (1983)

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

12.2.9 Volatilization from Water/Soil



The Henry's Law constant for dibutyl sebacate is estimated as 4.8×10^{-8} atm-cu m/mole(SRC) from its vapor pressure, 4.7X10-6 mm Hg(1), and [water](#) solubility, 40 mg/l(2). This Henry's Law constant indicates that dibutyl sebacate is expected to be essentially nonvolatile from [water](#) surfaces(3). Dibutyl sebacate's estimated Henry's Law constant(1,2) indicates that volatilization from moist soil surfaces is not expected to be an important environmental fate process(SRC). Volatilization from dry soil surfaces is not expected to be an important fate process(SRC) based on the vapor pressure of this compound(1).

(1) Daubert TE, Danner RP; *Physical and Thermodynamic Properties of Pure Chemicals Data Compilation Washington, DC: Taylor and Francis (1996)* (2) Riddick JA et al; *Organic Solvents: Physical Properties and Methods of Purification. 4th ed NY, NY: Wiley Interscience (1986)* (3) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)*

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

12.2.10 Environmental Water Concentrations



Dibutyl sebacate was identified, not quantified, in drinking [water](#) from the US(1).

(1) Lucas SV; *GC/MS Analysis of Drinking Water Concentrates and Advanced Waste Treatment Concentrates. Vol 1: Analysis Results for 17 Drinking Water, 16 Advanced Waste Treatment and 3 Process Blank Concentrates. Columbus, OH: USEPA-600/1-84-20b, NTIS PB85-128239 (1984)*

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

12.2.11 Probable Routes of Human Exposure



NIOSH (NOES Survey 1981-1983) has statistically estimated that 4,826 workers (2,128 of these are female) are potentially exposed to dibutyl sebacate in the US(1). Occupational exposure to dibutyl sebacate may occur through inhalation and dermal contact with this compound at workplaces where dibutyl sebacate is produced or used(SRC). The general population is exposed to dibutyl sebacate through the use of consumer products that contain this compound(SRC).

(1) NIOSH; *National Occupational Exposure Survey (NOES) (1983)*

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

13 Literature



13.1 NLM Curated PubMed Citations



► PubChem

13.2 Springer Nature References



► Springer Nature

13.3 Depositor Provided PubMed Citations



► PubChem

13.4 Metabolite References



▶ Human Metabolome Database (HMDB)

13.5 Chemical Co-Occurrences in Literature



▶ PubChem

13.6 Chemical-Gene Co-Occurrences in Literature



▶ PubChem

13.7 Chemical-Disease Co-Occurrences in Literature



▶ PubChem

14 Patents



14.1 Depositor-Supplied Patent Identifiers



▶ PubChem

[Link to all deposited patent identifiers](#)

▶ PubChem

14.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

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

▶ PATENTSCOPE (WIPO)

15 Biological Test Results



15.1 BioAssay Results



► PubChem

16 Classification



16.1 Ontologies



16.1.1 MeSH Tree



► Medical Subject Headings (MeSH)

16.1.2 EPA Safer Choice



► EPA Safer Choice

16.1.3 ChemIDplus



► ChemIDplus

16.1.4 UN GHS Classification



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

16.1.5 EPA CPDat Classification



▶ EPA Chemical and Products Database (CPDat)

16.1.6 NORMAN Suspect List Exchange Classification



▶ NORMAN Suspect List Exchange

16.1.7 EPA DSSTox Classification



▶ EPA DSSTox

17 Information Sources



FILTER BY SOURCE ALL SOURCES

- ### 1. ChemIDplus

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<https://www.nlm.nih.gov/copyright.html>

Dibutyl sebacate [NF]
<https://chem.nlm.nih.gov/chemidplus/sid/0000109433>

ChemIDplus Chemical Information Classification
<https://chem.nlm.nih.gov/chemidplus/>
- ### 2. DTP/NCI

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<https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=3893>
- ### 3. EPA Chemicals under the TSCA

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<https://www.epa.gov/chemicals-under-tsca>
- ### 4. EPA DSSTox

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Dibutyl decanedioate
<https://comptox.epa.gov/dashboard/DTXSID1041847>

CompTox Chemicals Dashboard Chemical Lists
https://comptox.epa.gov/dashboard/chemical_lists/
- ### 5. European Chemicals Agency (ECHA)

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<https://echa.europa.eu/web/guest/legal-notice>

Dibutyl sebacate
<https://echa.europa.eu/substance-information/-/substanceinfo/100.003.339>

Dibutyl sebacate
<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/74146>
- ### 6. Hazardous Substances Data Bank (HSDB)

DIBUTYL SEBACATE
<https://pubchem.ncbi.nlm.nih.gov/source/hsdb/309>
- ### 7. Human Metabolome Database (HMDB)

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HMDB is offered to the public as a freely available resource. Use and re-distribution of the data, in whole or in part, for commercial purposes requires explicit permission of the authors and explicit acknowledgment of the source material (HMDB) and the original publication (see the HMDB citing page). We ask that users who download significant portions of the database cite the HMDB paper in any resulting publications.
<http://www.hmdb.ca/citing>

Dibutyl decanedioate
<http://www.hmdb.ca/metabolites/HMDB0041220>
- ### 8. ILO International Chemical Safety Cards (ICSC)

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DIBUTYL SEBACATE
https://www.ilo.org/dyn/icsc/showcard.display?p_version=2&p_card_id=1349
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Sebacic acid, dibutyl ester
<https://www.cdc.gov/niosh-rtecs/VST18C30.html>
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<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

dibutyl sebacate
<https://comptox.epa.gov/dashboard/DTXSID1041847#exposure>

EPA CPDat Classification
<https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat>
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Dibutyl sebacate

<http://www.fao.org/food/food-safety-quality/scientific-advice/jecfa/jecfa-flav/details/en/c/1118/>

BUTYL SEBACATE

<https://apps.who.int/food-additives-contaminants-jecfa-database/chemical.aspx?chemID=1308>

12. EPA Safer Choice

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

Dibutyl sebacate

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

EPA Safer Chemical Ingredients Classification

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

13. EU Food Improvement Agents

Dibutyl sebacate

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

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NORMAN Suspect List Exchange Classification

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

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DIBUTYL SEBACATE

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

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<https://www.fda.gov/about-fda/about-website/website-policies#linking>

4WSIH7FLNY

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

17. Flavor and Extract Manufacturers Association (FEMA)

DIBUTYL SEBACATE

<https://www.femaflavor.org/flavor-library/dibutyl-sebacate>

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<https://foodb.ca/about>

Dibutyl decanedioate

<https://foodb.ca/compounds/FDB021119>

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<https://mona.fiehnlab.ucdavis.edu/documentation/license>

DECANEDIOIC ACID DIBUTYL ESTER

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

20. NIST Mass Spectrometry Data Center

Decanedioic acid, dibutyl ester

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

21. SpectraBase

Dibutyl sebacate

<https://spectrabase.com/spectrum/AmvKQXp9p1>

Butyl sebacate

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

Dibutyl sebacate

<https://spectrabase.com/spectrum/9Vml98qhtzT>

DIBUTYL SEBACATE

<https://spectrabase.com/spectrum/19z5Oym1853>

DIBUTYL SEBACATE

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

DIBUTYL SEBACATE

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

BUTYL SEBACATE

<https://spectrabase.com/spectrum/6Vrslt0YUnR>

SEBACIC ACID, DIBUTYL ESTER

<https://spectrabase.com/spectrum/3KuuyJT6HGV>

SEBACIC ACID, DIBUTYL ESTER

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

Decanedioic acid, dibutyl ester; Di-butyl sebacate; Sebacic acid, dibutyl ester

<https://spectrabase.com/spectrum/1jkkx3IN7Ay>

dibutyl sebacate

<https://spectrabase.com/spectrum/8j5E8AP96P5>

SEBACIC ACID, DIBUTYL ESTER

<https://spectrabase.com/spectrum/9MMtC5Vp6v>

SEBACIC ACID, DIBUTYL ESTER

<https://spectrabase.com/spectrum/9Pz8XPok5Tk>

Sebacic acid, dibutyl ester

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

sebacic acid, dibutyl ester

<https://spectrabase.com/spectrum/8KaHODIVv4k>

Decanedioic acid, dibutyl ester

<https://spectrabase.com/spectrum/eWwyP9W9pO>

Decanedioic acid, dibutyl ester

<https://spectrabase.com/spectrum/DlmX4Rz0Suy>

<https://spectrabase.com/spectrum/Gx8Ec63kJvD>

Dibutyl sebacate

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

Dibutyl sebacate

<https://spectrabase.com/spectrum/9zSBN8eV6AK>

Decanedioic acid, dibutyl ester

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

Decanedioic acid, dibutyl ester

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

Decanedioic acid, dibutyl ester

<https://spectrabase.com/spectrum/1o6SK7NwErI>

Decanedioic acid, dibutyl ester

<https://spectrabase.com/spectrum/JxCn5teW9YW>

Decanedioic acid, dibutyl ester

<https://spectrabase.com/spectrum/7WSzTvdb8qFU>

Decanedioic acid, dibutyl ester

<https://spectrabase.com/spectrum/Ddu41Xp8pEW>

22. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/341176281>

23. Wikipedia

dibutyl sebacate

https://en.wikipedia.org/wiki/Dibutyl_sebacate

24. PubChem

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

25. MeSH

dibutyl sebacate

<https://www.ncbi.nlm.nih.gov/mesh/67055481>

26. Medical Subject Headings (MeSH)

MeSH Tree

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

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

GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

28. PATENTSCOPE (WIPO)

SID 403410909

<https://pubchem.ncbi.nlm.nih.gov/substance/403410909>