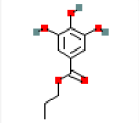
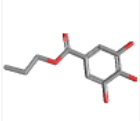
PubChem

COMPOUND SUMMARY

Propyl gallate

PubChem CID	4947
Structure	 2D  3D Find Similar Structures
Chemical Safety	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{10}H_{12}O_5$
Synonyms	propyl gallate 121-79-9 Propyl 3,4,5-trihydroxybenzoate N-Propyl gallate Tenox PG More...
Molecular Weight	212.2 g/mol
Dates	Modify 2020-11-07 Create 2005-03-25

Propyl gallate appears as fine white to creamy-white crystalline powder. Odorless or with a faint odor. Melting point 150°C. Insoluble in water. Slightly bitter taste.

▸ CAMEO Chemicals

N-propyl gallate is a trihydroxybenzoic acid.

▸ ChEBI

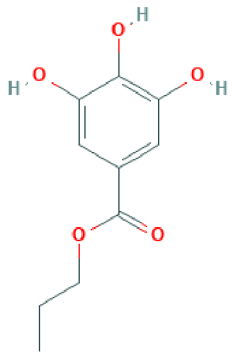
Propyl Gallate is under investigation in clinical trial NCT01450098 (A Study of LY2484595 in Healthy Subjects).

▸ DrugBank

1 Structures

1.1 2D Structure

Chemical Structure Depiction

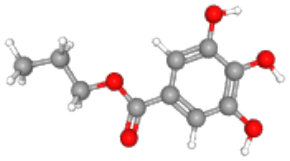


PubChem

1.2 3D Conformer

Interactive Chemical Structure Model

- (•) Ball and Stick
- ( ) Sticks
- ( ) Wire-Frame
- ( ) Space-Filling
- [x] Show Hydrogens
- [ ] Animate



PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

propyl 3,4,5-trihydroxybenzoate

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

PubChem

2.1.2 InChI

InChI=1S/C10H12O5/c1-2-3-15-10(14)6-4-7(11)9(13)8(12)5-6/h4-5,11-13H,2-3H2,1H3

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

2.1.3 InChI Key

ZTHYODDOHIVTJV-UHFFFAOYSA-N

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

2.1.4 Canonical SMILES

CCCOC(=O)C1=CC(=C(C(=C1)O)O)O

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

PubChem

2.2 Molecular Formula

C10H12O5

EU Food Improvement Agents; PubChem

2.3 Other Identifiers

2.3.1 CAS

121-79-9

CAMEO Chemicals; ChemIDplus; DrugBank; 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

56274-95-4

ChemIDplus

2.3.3 European Community (EC) Number

204-498-2

EU Food Improvement Agents; European Chemicals Agency (ECHA)

2.3.4 NSC Number

2626

DTP/NCI

2.3.5 UNII

8D4SNN7V92

FDA/SPL Indexing Data

2.3.6 FEMA Number

2947

Flavor and Extract Manufacturers Association (FEMA)

2.3.7 DSSTox Substance ID

DTXSID5021201

EPA DSSTox

2.3.8 Wikipedia

Propyl gallate

Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

Gallate, Propyl
Propyl Gallate

MeSH

2.4.2 Depositor-Supplied Synonyms

propyl gallate	3,4,5-Trihydroxybenzoic acid propyl ester	CCRIS 541	8D4SNN7V92	CAS-121-79-9	Oprea1_
121-79-9	Propylester kyseliny gallove	Nipanox S 1	CHEBI:10607	n-Propyl-3,4,5-Trihydroxybenzoate	SCHEME
Propyl 3,4,5-trihydroxybenzoate	n-Propyl ester of 3,4,5-trihydroxybenzoic acid	HSDB 591	NSC2626	Propylgallate	CBDivE_
N-Propyl gallate	n-Propyl 3,4,5-trihydroxybenzoate	Propyl gallate (NF)	NSC-2626	Propyl galiate	KSC175K
Tenox PG	FEMA No. 2947	Propyl gallate [NF]	MFCD00002196	n-propyl-gallate	BIDD:ER
Progallin P	Pro gallin P	Propyl gallate, 98%	NCGC00164234-01	Sustane PG	Propyl 3
Nipagallin P	Gallic acid n-propyl ester	EINECS 204-498-2	AK-94176	Propylgallate,(S)	WLN: QI
Gallic acid, propyl ester	NSC 2626	Propylester kyseliny gallove [Czech]	DSSTox_CID_1201	Propyl Gallate FCC	INS NO.
Gallic acid propyl ester	3,4,5-Trihydroxybenzoic acid, propyl ester	CHEMBL7983	DSSTox_RID_76009	Propyl gallate, powder	DTXSID5
NIPA 49	NCI-C505888	Gallic acid, n-propyl ester	DSSTox_GSID_21201	ACMC-209ahq	CTK0H5
Benzoic acid, 3,4,5-trihydroxy-, propyl ester	3,4,5-Trihydroxybenzoic acid n-propyl ester	E310	Q-201634	Gallic acid-propyl ester	FEMA 2
3,4,5-Trihydroxybenzene-1-propylcarboxylate	UNII-8D4SNN7V92	AI3-17136	Gallate, Propyl	3,4,5-Trihydroxy-benzoic acid propyl ester	KS-0000

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	212.2 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
XLogP3	1.8	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	3	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	5	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	4	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	212.068473 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Monoisotopic Mass	212.068473 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Topological Polar Surface Area	87 Å²	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	15	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	206	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

Propyl gallate appears as fine white to creamy-white crystalline powder. Odorless or with a faint odor. Melting point 150°C. Insoluble in water. Slightly bitter taste.

CAMEO Chemicals

DryPowder

EPA Chemicals under the TSCA

White to creamy-white, crystalline, odourless solid

EU Food Improvement Agents

Solid

Human Metabolome Database (HMDB)

3.2.2 Color/Form

White to creamy-white crystalline powder

Osol, A. and J.E. Hoover, et al. (eds.). Remington's Pharmaceutical Sciences. 15th ed. Easton, Pennsylvania: Mack Publishing Co., 1975., p. 1223

Hazardous Substances Data Bank (HSDB)

Colorless crystals

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; Hawley's Condensed Chemical Dictionary 16th Edition. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 1143

Hazardous Substances Data Bank (HSDB)

Needles in water

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-470

Hazardous Substances Data Bank (HSDB)

Fine, ivory powder or crystals

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 3792

Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

Odorless

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 3792

Hazardous Substances Data Bank (HSDB)

Odorless or with a faint odor

NOAA; CAMEO Chemicals. Database of Hazardous Materials. Propyl Gallate (121-79-9). Natl Ocean Atmos Admin, Off Resp Rest; NOAA Ocean Serv. Available from, as of Oct 21, 2016: ***http://cameochemicals.noaa.gov/***

Hazardous Substances Data Bank (HSDB)

3.2.4 Taste

Slightly bitter taste

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 3792

Hazardous Substances Data Bank (HSDB)

3.2.5 Boiling Point

Decomposes (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

3.2.6 Melting Point

302 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

130.0 °C

EPA DSSTox

Between 146 °C and 150 °C after drying at 110 °C for four hours

EU Food Improvement Agents

Mp 150 ° (147-148 °)

DFC

FooDB

147-149 °C

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 3792

Hazardous Substances Data Bank (HSDB)

150°C

Human Metabolome Database (HMDB)

3.2.7 Flash Point

368 °F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

187 °C (369 °F) - closed cup

Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: ***http://www.sigmaaldrich.com/safety-center.html***

Hazardous Substances Data Bank (HSDB)

3.2.8 Solubility

less than 1 mg/mL at 68° F (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

0.02 M

MERCK INDEX (1996)

EPA DSSTox

Slightly soluble in **water**, freely soluble in **ethanol**, ether and **propane-1,2-diol**

EU Food Improvement Agents

3.5 mg/mL at 25 °C

MERCK INDEX (1996)

- FooDB; Human Metabolome Database (HMDB)

In water, 3490 mg/L at 25 deg, 2790 mg/L at 20 °C, 3790 mg/L at 30 °C

Yalkowsky, S.H., He, Yan, Jain, P. Handbook of Aqueous Solubility Data Second Edition. CRC Press, Boca Raton, FL 2010, p. 690

- Hazardous Substances Data Bank (HSDB)

Solubility at 25 °C: in water 0.35 g/100 mL

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1455

- Hazardous Substances Data Bank (HSDB)

Slightly soluble in acetone and 2-butanol

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 12th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2012., p. 3792

- Hazardous Substances Data Bank (HSDB)

Solubility at 25 °C: in alcohol 103 g/100 g, in ether 83 g/100 g; Solubility at 30 °C: in cottonseed oil at 30 °C 1.23 g/100 g, in lard at 45 °C 1.14 g/100 g

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1455

- Hazardous Substances Data Bank (HSDB)

3.2.9 Density

1.21 (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

1.21

NOAA; CAMEO Chemicals. Database of Hazardous Materials. Propyl Gallate (121-79-9). Natl Ocean Atmos Admin, Off Resp Rest; NOAA Ocean Serv. Available from, as of Oct 21, 2016: http://cameochemicals.noaa.gov/

- Hazardous Substances Data Bank (HSDB)

3.2.10 Vapor Density

7.3 (NTP, 1992) (Relative to Air)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

- CAMEO Chemicals

3.2.11 Vapor Pressure

2.6X10-7 mm Hg at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: http://www2.epa.gov/tsca-screening-tools

- Hazardous Substances Data Bank (HSDB)

3.2.12 LogP

1.8 (LogP)

HANSCH,C ET AL. (1995)

- EPA DSSTox

1.80

HANSCH,C ET AL. (1995)

- FooDB; Human Metabolome Database (HMDB)

log Kow = 1.80

Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 73

- Hazardous Substances Data Bank (HSDB)

3.2.13 Stability/Shelf Life

Stable under recommended storage conditions.

Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: 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 fumes.

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3084

Hazardous Substances Data Bank (HSDB)

3.2.15 pH

pH = 6.3 (0.05% aqueous solution); pH = 5.9 (0.1% aqueous solution); pH = 5.7 (0.2% aqueous solution)

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1455

Hazardous Substances Data Bank (HSDB)

3.2.16 Dissociation Constants

pKa = 7.94

Shahidi F, ed; Handbook of Antioxidants for Food Preservation. Waltham, MA: Woodhead Publishing, p. 54 (2015)

Hazardous Substances Data Bank (HSDB)

3.2.17 Other Experimental Properties

Darkens in presence of iron and iron salts

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1455

Hazardous Substances Data Bank (HSDB)

Synergic with acids, BHA, BHT

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1455

Hazardous Substances Data Bank (HSDB)

Propyl gallate can react with oxidizing agents. Incompatible with strong acids, strong bases and strong reducing agents.

*NOAA; CAMEO Chemicals. Database of Hazardous Materials. Propyl Gallate (121-79-9). Natl Ocean Atmos Admin, Off Resp Rest; NOAA Ocean Serv. Available from, as of Oct 21, 2016: **http://cameochemicals.noaa.gov/***

Hazardous Substances Data Bank (HSDB)

Henry's Law constant = 2.1X10-11 atm-cu m/mol at 25 °C /Estimated from vapor pressure and water solubility/

*US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: **http://www2.epa.gov/tsca-screening-tools***

Hazardous Substances Data Bank (HSDB)

Hydroxyl radical reaction rate constant = 9.2X10-11 cu cm/molecule-sec at 25 °C (est)

*US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: **http://www2.epa.gov/tsca-screening-tools***

Hazardous Substances Data Bank (HSDB)

4 Spectral Information

4.1 1D NMR Spectra

Showing 2 of 3 View More

1D NMR Spectra	NMR: 18733 (Sadtler Research Laboratories Spectral Collection)

▶ Hazardous Substances Data Bank (HSDB)

1D NMR Spectra	1D NMR Spectrum 2883 - Propyl gallate (HMDB0033835)

▶ Human Metabolome Database (HMDB)

4.1.1 1H NMR Spectra

Instrument Name	Varian A-60D
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ SpectraBase

4.1.2 13C NMR Spectra

Source of Sample	Eastman Organic Chemicals, Rochester, New York
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ SpectraBase

Copyright	Copyright © 2016 W. Robien, Inst. of Org. Chem., Univ. of Vienna. All Rights Reserved.
Thumbnail	

SpectraBase

4.2 Mass Spectrometry

4.2.1 GC-MS

Showing 2 of 5 View More

GC-MS	GC-MS Spectrum 1744 - Propyl gallate (HMDB0033835) GC-MS Spectrum 31632 - Propyl gallate (HMDB0033835)

Human Metabolome Database (HMDB)

MoNA ID	HMDB0033835_c_ms_1744
MS Category	Experimental
MS Type	GC-MS
Instrument Type	GC-MS
Splash	splash10-003r-1591200000-83ddc9d65f8d1fc4dc59
Thumbnail	
Submitter	David Wishart, University of Alberta

MassBank of North America (MoNA)

4.2.2 MS-MS

NIST Number	1118559
Instrument Type	IT/ion trap
Collision Energy	0
Spectrum Type	MS2
Precursor Type	[M-H]-
Precursor m/z	211.0612
Total Peaks	8
m/z Top Peak	169.1
m/z 2nd Highest	168.1
m/z 3rd Highest	124.1
Thumbnail	

NIST Mass Spectrometry Data Center

NIST Number	1118560
Instrument Type	IT/ion trap
Collision Energy	0
Spectrum Type	MS2
Precursor Type	[M+H]+
Precursor m/z	213.0757
Total Peaks	5
m/z Top Peak	171.2
m/z 2nd Highest	127.1
m/z 3rd Highest	153.2
Thumbnail	

NIST Mass Spectrometry Data Center

4.2.3 LC-MS

Showing 2 of 5 View More

MoNA ID	LU032351
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M-H]-
precursor m/z	211.0612
Instrument	Q Exactive Orbitrap (Thermo Scientific)
Instrument Type	LC-ESI-QFT
Ionization	ESI
Ionization Mode	negative
Retention Time	14.149 min
Splash	splash10-03di-0190000000-d7a6b4a1c39f76236649
Thumbnail	
Submitter	Anjana Elapavalore, Environmental Cheminformatics, LCSB, University of Luxembourg

MassBank of North America (MoNA)

MoNA ID	LU032352
MS Category	Experimental
MS Type	LC-MS

MS Level	MS2
Precursor Type	[M-H]-
precursor m/z	211.0612
Instrument	Q Exactive Orbitrap (Thermo Scientific)
Instrument Type	LC-ESI-QFT
Ionization	ESI
Ionization Mode	negative
Retention Time	14.149 min
Splash	splash10-03di-0490000000-502ac5be04c11da5d505
Thumbnail	
Submitter	Anjana Elapavalore, Environmental Cheminformatics, LCSB, University of Luxembourg

MassBank of North America (MoNA)

4.2.4 EI-MS

EI-MS	EI-MS Spectrum 991 - Propyl gallate (HMDB0033835)

Human Metabolome Database (HMDB)

4.2.5 Other MS

Other MS	MASS: 70022 (NIST/EPA/MSDC Mass Spectral Database, 1990 Version)

Hazardous Substances Data Bank (HSDB)

4.3 UV Spectra

Max absorption (alcohol): 275 nm; 9163 (IR, Prism)

Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-199

Hazardous Substances Data Bank (HSDB)

The UV spectrum of propyl gallate in water has two characteristic bands: maximum #1 at 217 nm and maximum #2 at 274 nm

Szymula M; J Cosmet Sci 55: 281-289 (2004). Available from, as of Oct 24, 2016: http://journal.scconline.org/pdf/cc2004/cc055n03/p00281-p00289.pdf

Hazardous Substances Data Bank (HSDB)

4.3.1 UV-VIS Spectra

Copyright	Copyright © 2008-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.4 IR Spectra

IR Spectra	IR: 2023 (Coblentz Society Spectral Collection)

Hazardous Substances Data Bank (HSDB)

4.4.1 FTIR Spectra

Showing 2 of 8 View More

Technique	BETWEEN SALTS
Source of Sample	The Harshaw Chemical Company
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Technique	KBr WAFER
Source of Sample	Eastman Chemcial Products, Inc., Kingsport, Tennessee
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.4.2 ATR-IR Spectra

Instrument Name	Bruker Tensor 27 FT-IR
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Alfa Aesar, Thermo Fisher Scientific
Catalog Number	A10877
Lot Number	10158862
Copyright	Copyright © 2016-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.4.3 Vapor Phase IR Spectra

Instrument Name	DIGILAB FTS-14
Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.5 Raman Spectra

Instrument Name	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
Technique	FT-Raman
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Alfa Aesar, Thermo Fisher Scientific
Catalog Number	A10877
Lot Number	10158862
Copyright	Copyright © 2016-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

PubChem

5.2 Related Compounds

Same Connectivity	2 Records
Same Parent, Connectivity	19 Records
Same Parent, Exact	18 Records
Mixtures, Components, and Neutralized Forms	55 Records
Similar Compounds	1,277 Records
Similar Conformers	747 Records

PubChem

5.3 Substances

5.3.1 Related Substances

All	241 Records
Same	174 Records
Mixture	67 Records

PubChem

5.3.2 Substances by Category

PubChem

5.4 Entrez Crosslinks

PubMed	357 Records
Taxonomy	6 Records
OMIM	1 Record
Gene	24 Records

PubChem

6 Chemical Vendors

PubChem

7 Drug and Medication Information

7.1 Therapeutic Uses

/EXPL THER/ In addition to the hepatocellular edema and cytoplasmic eosinophilia, sludging of blood was present in liver of mice exposed to trinitrotoluene (TNT). Single necrosis of the partical liver cell was seen occasionally. Liver damage induced by TNT was significantly alleviated by orally administrated propyl gallate (PG). Futhermore, PG can promote the regeneration of the hepatocytes following TNT-exposed mice. The results suggest that PG showed a protective effect on the histopathologic changes of liver injury induced by TNT.

PMID:10684118
Li Z et al; Wei Sheng Yan Jiu 27 (3): 151-3 (1998)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ Phosgene, widely used in industrial processes, can cause life-threatening pulmonary edema and acute lung injury. One mechanism of protection against phosgene-induced lung injury may involve the use of antioxidants. The present study focused on dietary supplementation in mice using n-propyl gallate (nPG)--a gallate acid ester compound used in food preservation--and vitamin E. Five groups of male mice were studied: group 1, control-fed with Purina rodent chow 5002; group 2, fed 0.75% nPG (w/w) in 5002; group 3, fed 1.5% nPG (w/w) in 5002; group 4 fed 1% (w/w) vitamin E in 5002; and group 5, fed 2% (w/w) vitamin E also in 5002. Mice were fed for 23 days. On day 23 mice were exposed to 32 mg m-3 (8 ppm) phosgene for 20 min (640 mg. min m-3) in a whole-body exposure chamber. Survival rates were determined at 12 and 24 hr. In mice that died within 12 h, the lungs were removed and lung wet weights, dry weights, wet/dry weight ratios, lipid peroxidation (thiobarbituric acid reactive substances, TBARS) and glutathione (GSH) were assessed. Vitamin E had no positive effect on any outcome measured. There was no significant difference between 1.5% nPG and any parameter measured or survival rate compared with 5002 + phosgene. However, dietary treatment with 0.75% nPG significantly increased survival rate (p

PMID:11180278
Sciuto AM, Moran TS; J Appl Toxicol 21 (1): 33-9 (2001)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ ... In the present study we explored the role of oxidants present in ambient particles in causing damage to the mucociliary epithelium. We explored the protective effects of pretreatment with three substances (n-propyl gallate, DL-alpha-tocopherol acetate, and EDTA) on the frog palate exposed to residual oil fly ash (ROFA). The parameters analyzed were mucociliary transport (MCT) and ciliary beating frequency (CBF) after 0, 10, 20, 30, 60, and 120 min of exposure. MCT was decreased significantly by ROFA ($p<0.001$), with a significant interaction effect ($p=0.02$) between the duration of exposure and treatment with antioxidants. The inhibitory effects on MCT of the substances tested were significantly different ($p=0.002$); vitamin E was similar to control (Ringer) and different from all other groups. CBF showed no significant effect of duration of exposure ($p=0.465$), but a significant interaction between duration of exposure and treatments was observed ($p=0.011$). Significant differences were detected among treatments ($p<0.001$), with ROFA and n-propyl gallate at concentrations of 50 uM presenting a short-lived increase in CBF, which was not observed in the remaining groups. The results showed that both MCT and CBF were affected within a short period (100 min) of exposure to ROFA and that the presence of antioxidant substances, such as vitamin E (4 mg/mL) and n-propyl gallate (300 uM), protected against the mucociliary impairment induced by ROFA on the frog palate.

PMID:15910789
Carvalho-Oliveira R et al; Environ Res 98 (3): 349-54 (2005)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ Ca(2+) sensitizers are cardiotonic agents that directly increase the Ca(2+) sensitivity of cardiac myofilament. To find a novel Ca(2+) sensitizer, we have screened a group of phenolic compounds by examining their effects on the Ca(2+)-dependent force generation in cardiac muscle fibers. We found that propyl gallate, a strong antioxidant, increased the Ca(2+) sensitivity of cardiac myofilament in a dose-dependent and reversible manner. The present study indicates that propyl gallate is a novel type of Ca(2+) sensitizer with antioxidant activity, which might be more beneficial for the treatment of congestive heart failure associated with oxidative stress than existing Ca(2+) sensitizers.

PMID:19305124
Tadano N et al; J Pharmacol Sci 109 (3): 456-8 (2009)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ ... In the present study, we demonstrated ... that pure polyphenols such as gallic acid, ferulic acid, caffeic acid, coumaric acid,propyl gallate, epicatechin, epigallocatechin, and epigallocatechin gallate protect, rescue and, most importantly, restore the impaired movement activity (i.e., climbing capability) induced by paraquat in Drosophila melanogaster, a valid model of Parkinson's disease (PD). We also showed for the first time that high concentrations of iron (e.g. 15 mM FeSO(4)) are able to diminish fly survival and movement to a similar extent as (20 mM) paraquat treatment. Moreover, paraquat and iron synergistically affect both survival and locomotor function. ... Propyl gallate and epigallocatechin gallate protected and maintained movement abilities in flies co-treated with paraquat and iron. Our findings indicate that pure polyphenols might be potent neuroprotective agents for the treatment of PD against stressful stimuli.

PMID:19701790
Jimenez-Del-Rio M et al; Neurochem Res 35 (2): 227-38 (2010)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ In mammals, aging is linked to a decline in the activity of citrate synthase (CS; E.C. 2.3.3.1), the first enzyme of the citric acid cycle. We used 2,2'-azobis(2-amidinopropane) dihydrochloride (AAPH), a water-soluble generator of peroxyl and alkoxyl radicals, to investigate the susceptibility of CS to oxidative damage. Treatment of isolated mitochondria with AAPH for 8-24 hr led to CS inactivation; however, the activity of aconitase, a mitochondrial enzyme routinely used as an oxidative stress marker, was unaffected. In addition to enzyme inactivation, AAPH treatment of purified CS resulted in dityrosine formation, increased protein surface hydrophobicity, and loss of tryptophan fluorescence. Propyl gallate, 1,8-naphthalenediol, 2,3-naphthalenediol, ascorbic acid, glutathione, and oxaloacetate protected CS from AAPH-mediated inactivation, with IC(50) values of 9, 14, 34, 37, 150, and 160 uM, respectively. Surprisingly, the antioxidant epigallocatechin gallate offered no protection against AAPH, but instead caused CS inactivation. Our results suggest that the current practice of using the enzymatic activity of CS as an index of mitochondrial abundance and the use of aconitase activity as an oxidative stress marker may be inappropriate, especially in oxidative stress-related studies, during which alkyl peroxyl and alkoxyl radicals can be generated.

PMID:19795928
Chepelev NL et al; J Enzyme Inhib Med Chem 24 (6): 1319-31 (2009)

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ There is ... evidence suggesting that glomerular endothelial cell proliferation and angiogenesis may be responsible for the pathophysiological events in the early stage of diabetic nephropathy. This study was designed to investigate the factors related to glomerular endothelial cell proliferation and glomerular angiogenesis and assess the effect of propyl gallate on preventing these disorders in diabetic rats. We found that glomerular hypertrophy, glomerular mesangial matrix expansion, and albuminuria were significantly increased in DN rats. CD31+ endothelial cells significantly increased in glomerulus of diabetic rats. Double immunofluorescence staining showed some structurally defective vasculus tubes in glomerulus. Real-time PCR and western blot demonstrated the glomerular eNOS expression remained at the same level, while remarkable decreased NO productions and suppressed eNOS activities were observed in diabetic rats. Treatment with propyl gallate improved glomerular pathological changes, reduced endothelial cell proliferation, decreased albuminuria, and restored eNOS activity, but did not alter eNOS expression. These data suggest that endothelial cell proliferation and immature angiogenesis may be the contributors to progression of DN. Propyl gallate is a potential novel therapeutic agent on prevention of diabetic nephropathy.

PMID:22988451
Full text: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3439983
Tian S et al; Exp Diabetes Res 2012: 209567 doi: 10.1155/2012/209567 (2012) Epub 2012 Sep 4

Hazardous Substances Data Bank (HSDB)

/EXPL THER/ Hepatic stellate cells (HSCs) play a central role in liver fibrosis. Inhibition of HSC growth and induction of apoptosis have been proposed as therapeutic strategies for the treatment and prevention of liver fibrosis. ... In this study, we investigated whether propyl gallate (PG) could induce apoptosis in activated HSCs. Treatment of activated HSCs with PG inhibited cell viability in a dose- and time-dependent manner. PG induced apoptosis as demonstrated by morphological changes, poly(ADP-ribose) polymerase (PARP) cleavage, caspase-3 cleavage, increased Bad expression, and decreased Bcl-2 protein expression. Through stimulation of the activation of c-Jun NH2-terminal protein kinase (JNK) and p38 mitogen-activated protein kinases (MAPK) by PG treatment, we demonstrated that JNK and p38 MPAK are not involved in PG-induced apoptosis using their specific inhibitors. Taken together, these findings indicate that PG induces apoptosis in activated HSCs. ...

PMID:23263816

Che XH et al; Arch Pharm Res 35 (12): 2205-10 (2012)

Hazardous Substances Data Bank (HSDB)

8 Food Additives and Ingredients

8.1 Food Additive Classes

JECFA Functional Classes

Food Additives -> ANTIOXIDANT

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

8.2 FDA Substances Added to Food

Substance	PROPYL GALLATE
Used for (Technical Effect)	FLAVORING AGENT OR ADJUVANT
Document Number (21 CFR)	172.615 175.125 175.300 175.380 175.390 176.170 177.1010 177.1210 177.1350 181.24 184.1660

▸ FDA Center for Food Safety and Applied Nutrition (CFSAN)

8.3 Organoleptic Properties

Flavors

bitter

bland

▸ FooDB

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

Chemical Name	PROPYL GALLATE
Evaluation Year	1996
ADI	0-1.4 mg/kg bw (1993)
Comments	The 1993 ADI was maintained at the forty-sixth meeting (1996)
Report	TRS 868-JECFA 46/15

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

9 Pharmacology and Biochemistry

9.1 MeSH Pharmacological Classification

Antioxidants

Naturally occurring or synthetic substances that inhibit or retard oxidation reactions. They counteract the damaging effects of oxidation in animal tissues. (See all compounds classified as Antioxidants.)

▸ MeSH

9.2 Absorption, Distribution and Excretion

Propyl gallate was quickly metabolized and excreted when administered orally to rats and rabbits. ...When fed to rats, most of the propyl gallate was passed in the feces as the original ester. The urinary components detected were the original ester and gallic acid, and these were excreted completely within 24 hours. When administered orally to rabbits, 79 percent of the administered dose of propyl gallate was excreted in the urine, 72 percent as 4-methoxygallic acid glucuronide and 6.7 percent as unconjugated phenolic compounds. Minor metabolites included pyrogallol (free and conjugated) and free 4-methoxy gallic acid.

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: https://www3.epa.gov/

▸ Hazardous Substances Data Bank (HSDB)

In rats, /SRP: some/ of an oral dose of propyl gallate is absorbed in the GI tract. In vivo, the gallate esters are hydrolized to gallic acid and free alcohol. Free alcohol is metabolized through the Krebs cycle, and most of the gallic acid is converted into 4-O-methyl gallic acid. Free gallic acid or a conjugated derivative of 4-O-methyl gallic acid is excreted in the urine. Significant amounts of unchanged esters are excreted in the feces of rats.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 731

▸ Hazardous Substances Data Bank (HSDB)

9.3 Metabolism/Metabolites

Propyl gallate was quickly metabolized and excreted when administered orally to rats and rabbits. ...When fed to rats, most of the propyl gallate was passed in the feces as the original ester. The urinary components detected were the original ester and gallic acid, and these were excreted completely within 24 hours. When administered orally to rabbits, 79 percent of the administered dose of propyl gallate was excreted in the urine, 72 percent as 4-methoxygallic acid glucuronide and 6.7 percent as unconjugated phenolic compounds. Minor metabolites included pyrogallol (free and conjugated) and free 4-methoxy gallic acid.

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: https://www3.epa.gov/

▸ Hazardous Substances Data Bank (HSDB)

In rats, /SRP: some/ of an oral dose of propyl gallate is absorbed in the GI tract. In vivo, the gallate esters are hydrolized to gallic acid and free alcohol. Free alcohol is metabolized through the Krebs cycle, and most of the gallic acid is converted into 4-O-methyl gallic acid. Free gallic acid or a conjugated derivative of 4-O-methyl gallic acid is excreted in the urine. Significant amounts of unchanged esters are excreted in the feces of rats. In pigs, the metabolism is similar to rats.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 731

▸ Hazardous Substances Data Bank (HSDB)

The available evidence indicates that the gallate esters are hydrolyzed in the body to gallic acid. Most of the gallic acid is converted into 4-O-methyl gallic acid. Free gallic acid or a conjugated derivative of 4-O-methyl gallic acid is excreted in the urine. Conjugation of the 4-O-methyl gallic acid with glucuronic acid was demonstrated ... .

International Programme on Chemical Safety/World Health Organization; Food Additives Series 32, Gallates (1993). Available from, as of October 10, 2016: http://www.inchem.org/documents/jecfa/jecmono/v32je02.htm

▸ Hazardous Substances Data Bank (HSDB)

In vitro incubations with propyl, octyl and dodecyl gallate were performed using homogenates of liver, mucosa of the small intestine, and contents of caecum/colon as a source of intestinal microflora. The various homogenates were incubated at 37 °C with the individual gallate esters. At various time points up to 24 hr, samples were taken and analyzed by HPLC. ... All test substances were extensively metabolized by the homogenate of the intestinal mucosa. ... Furthermore, the caecum and colon contents also showed a high metabolic capacity, especially towards propyl gallate. The amt of gallic acid detected in the incubations was always much smaller than the total decrease of the amt of ester. It seems likely that apart from hydrolysis of the ester bond, other biotransformation routes ... are of major importance for all three gallate esters.

International Programme on Chemical Safety/World Health Organization; Food Additives Series 32, Gallates (1993). Available from, as of October 10, 2016: http://www.inchem.org/documents/jecfa/jecmono/v32je02.htm

▸ Hazardous Substances Data Bank (HSDB)

9.4 Mechanism of Action

The present study aimed to assess anti-inflammatory activity and underlying mechanism of n-propyl gallate, the n-propyl ester of gallic acid. n-Propyl gallate was shown to contain anti-inflammatory activity using two experimental animal models, acetic acid-induced permeability model in mice, and air pouch model in rats. It suppressed production of nitric oxide and induction of inducible nitric oxide synthase and cyclooxygenase-2 in the lipopolysaccharide (LPS)-stimulated RAW264.7 macrophage cells. It was able to diminish reactive oxygen species level elevated in the LPS-stimulated RAW264.7 macrophage cells. It also suppressed gelatinolytic activity of matrix metalloproteinase-9 enhanced in the LPS-stimulated RAW264.7 macrophage cells. It inhibited inhibitory kappaB-aplha degradation and enhanced NF-kappaB promoter activity in the stimulated macrophage cells. It was able to suppress phosphorylation of c-Jun NH(2)-terminal kinase 1/2 (JNK1/2) and activation of c-Jun promoter activity in the stimulated macrophage cells. In brief, n-propyl gallate possesses anti-inflammatory activity via down-regulation of NF-kappaB and JNK pathways.

PMID:20689985
Jung HJ et al; Inflammation 34 (5): 352-61 (2011)

▸ Hazardous Substances Data Bank (HSDB)

... In the present study, we demonstrate that propyl gallate (PG) reduced cell viability in THP-1, Jurkat, and HL-60 leukemia cells and induced apoptosis in THP-1 cells. PG activated caspases 3, 8, and 9 and increased the levels of p53, Bax, Fas, and Fas ligand. PG activated mitogen-activated protein kinases (MAPKs), inhibited nuclear translocation of the nuclear factor erythroid 2-related factor 2 (Nrf-2) and induced intracellular glutathione (GSH) depletion. In addition, PG increased superoxide dismutase-1 expression and decreased intracellular levels of reactive oxygen species.

Our data show ... that an early event of PG-induced apoptosis is MAPKs/Nrf-2-mediated GSH depletion and that PG induced apoptosis via multiple pathways in human leukemia. PG might serve as a potential chemotherapeutic agent or food supplement for human leukemia patients.

PMID:21112369
Chen CH et al; Food Chem Toxicol 49 (2): 494-501 (2011)

▸ Hazardous Substances Data Bank (HSDB)

9.5 Human Metabolite Information

9.5.1 Cellular Locations

Cytoplasm
Extracellular

▸ Human Metabolome Database (HMDB)

10 Use and Manufacturing

10.1 Overview

IDENTIFICATION: Propyl gallate is a white to creamy-white crystalline powder. It is odorless or may have a faint odor and has a slightly bitter taste. Propyl gallate is very soluble in water. It occurs naturally in corn seeds. USE: Propyl gallate is an important commercial chemical (IUR) used as a preservative in foods and cosmetics, especially fats, oils and waxes. It is also used as a preservative in transformer oils, some pesticides and to stabilize synthetic vitamin A. The proposed limit for use in cosmetic products is 0.1%. EXPOSURE: Workers that use propyl gallate may breathe in vapors or have direct skin contact. The general population may be exposed by ingestion of food and dermal contact with cosmetics containing propyl gallate. If propyl gallate is released to the environment, it will be broken down in air. Propyl gallate released to air also will be in or on particles that eventually fall to the ground. It is expected to be broken down by sunlight. It will not move into air from moist soil and water surfaces. It is expected to move moderately through soil. It will be broken down by microorganisms, and is not expected to build up in fish. RISK: Skin irritation and allergic reactions have been observed in some people following direct skin contact. No additional data on the potential for propyl gallate to cause toxic effects in humans were available. Due to its long history as a food additive with no apparent toxic effects, and lack of toxic effects in laboratory animals fed low-to-moderate doses, the U.S. Food and Drug Administration considers propyl gallate a "GRAS" (generally recognized as safe) food additive. Therefore, is not expected to cause any toxicity in humans at levels found in food. Decreased weight and damage, anemia, and damage to the digestive track were observed in laboratory animals ingesting a high dose of propyl gallate in feed over time. No effects were observed at lower feeding. No toxic effects have been observed following skin application of propyl gallate. No evidence of infertility, abortion, or birth defects were observed in laboratory animals exposed to propyl gallate before and/or during pregnancy. Propyl gallate has not been clearly associated with cancer in laboratory animals following life-time exposure in feed. California Proposition 65 has determined that propyl gallate has a low potential to cause cancer in humans based on the inconclusive studies in laboratory animals. The potential for propyl gallate 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 14th Report on Carcinogens. (SRC)

*FOR MORE INFORMATION: (1) National Library of Medicine Hazardous Substances Data Bank. Available from, as of Oct 26, 2016: **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 Oct 26, 2106: **http://monographs.iarc.fr/ENG/Classification/index.php** (3) National Library of Medicine Household Products Database. Available from, as of Oct 26, 2016: / **http://hpd.nlm.nih.gov** (4) National Toxicology Program. Testing Status of Agents at NTP. TR-240. Available from, as of Oct 26, 2016: **http://ntp.niehs.nih.gov/** (5) National Toxicology Program. Fourteenth Report on Carcinogens. Available from, as of Nov 18, 2016: **http://ntp.niehs.nih.gov/pubhealth/roc/index.html** (6) National Library of Medicine PubMed. Available from, as of Oct 27, 2016: **http://www.ncbi.nlm.nih.gov/pubmed** (7) USEPA; Chemical Data Reporting (CDR). Non-confidential 2012 Chemical Data Reporting information on chemical production and use in the United States. Available from, as of Oct 26, 2016: **http://java.epa.gov/oppt_chemical_search/** (8) USEPA/IRIS Integrated Risk Information System. Available from, as of Oct 26, 2016: **http://www.epa.gov/iris/** (9) US FDA. Everything Added to Food in the United States (EAFUS). November 2011. Propyl gallate (121-79-9). Available from, as of Oct 26, 2016: **http://www.accessdata.fda.gov/scripts/fcn/fcnNavigation.cfm?rpt=eafusListing** (10) US FDA; SCOGS (Select Committee on GRAS Substances). SCOGS Opinion: Propyl Gallate. Available from, as of Nov 18, 2016: **http://www.accessdata.fda.gov/scripts/fdcc/index.cfm?set=SCOGS***

- Hazardous Substances Data Bank (HSDB)

10.2 Use Classification

Food additives

- EU Food Improvement Agents

Food Additives -> ANTIOXIDANT -> JECFA Functional Classes

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

Cosmetics -> Antioxidant

*S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) | **DOI:10.5281/zenodo.2624118***

- NORMAN Suspect List Exchange

10.3 Uses

EPA CPDat Chemical and Product Categories

- EPA Chemical and Products Database (CPDat)

Reported uses (ppm):

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

Food Category	Usual	Max.
Baked goods	0.00	0.03
Fats, oils	0.06	0.15
Meat products	0.03	0.10
Nut products	0.01	0.01
Snack foods	0.01	0.03

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed.Boca Raton, FL 2010, p. 1755

- Hazardous Substances Data Bank (HSDB)

It is used as an antioxidant for foods and cosmetics; especially fats, oils, emulsions, and waxes. It is also used in transformer oils and as a stabilizer for synthetic vitamin A.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 730

▸ Hazardous Substances Data Bank (HSDB)

Reactive peroxides in **povidone** often lead to degradation of oxidation-labile drugs. ... The antioxidants **ascorbic acid**, propyl gallate, and **sodium sulfite** reduced the peroxide concentration in **povidone** ... .

PMID:22109686

Narang AS et al; J Pharm Sci 101 (1): 127-39 (2012)

▸ Hazardous Substances Data Bank (HSDB)

Synthetic antioxidants commonly used in food include butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT), propyl gallate (PG), and **tert-butylhydroquinone (TBHQ)**.

Somosyi L; Food Additives. Kirk-Othmer Encyclopedia of Chemical Technology (1999-2016). John Wiley & Sons, Inc. Online Posting Date: June 15, 2015

▸ Hazardous Substances Data Bank (HSDB)

MEDICATION

▸ Hazardous Substances Data Bank (HSDB)

10.3.1 Industry Uses

Oxidizing/reducing agents

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

▸ EPA Chemicals under the TSCA

10.3.2 Consumer Uses

Cleaning and furnishing care products

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

▸ EPA Chemicals under the TSCA

10.4 Methods of Manufacturing

Propyl gallate is manufactured via a reaction of **n-propanol** with **3,4,5-trihydroxybenzoic acid**.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 730

▸ Hazardous Substances Data Bank (HSDB)

Produced commercially by the esterification of **gallic acid** with **propyl alcohol** followed by distillation to remove the excess alcohol.

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed.Boca Raton, FL 2010, p. 1755

▸ Hazardous Substances Data Bank (HSDB)

REACTION OF **N-PROPYL ALCOHOL** WITH **3,4,5-TRIHYDROXYBENZOIC ACID**

SRI

▸ Hazardous Substances Data Bank (HSDB)

10.5 Formulations/Preparations

Trade Names: NIPA 49; Nipagallin P; Progallin P; and Tenox PG.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 729

▸ Hazardous Substances Data Bank (HSDB)

The antioxidant formulations most commonly used in edible products contain various combinations of BHA, BHT, and/or propyl gallate together with **citric acid** in a suitable solvent.

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 202

▸ Hazardous Substances Data Bank (HSDB)

10.6 Consumption Patterns

APPROXIMATELY 80% AS AN ANTIOXIDANT IN FATS & OILS; THE REMAINDER AS AN ANTIOXIDANT IN SHORTENING, SALT, BREAKFAST CEREAL, LARD, CHEWING GUM BASE, CANDY, CHICKEN SOUP BASE, FLAVORED BEVERAGES, FROZEN MILK DESSERTS, & BAKERY PRODUCTS(EST)(1972)

SRI

▸ Hazardous Substances Data Bank (HSDB)

10.7 U.S. Production

Aggregated Product Volume (EPA CDR 2016)

25,000 - 100,000 lb

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

EPA Chemicals under the TSCA

(1972) 5.0X10+7 GRAMS (EST)

SRI

Hazardous Substances Data Bank (HSDB)

(1975) PROBABLY GREATER THAN 9.08X10+5 GRAMS

SRI

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: Benzoic acid, 3,4,5-trihydroxy-, propyl ester. National Production Volume: 232,076 lb/yr.

USEPA/Pollution Prevention and Toxics; 2012 Chemical Data Reporting Database. Benzoic acid, 3,4,5-trihydroxy-, propyl ester (121-79-9). Available from, as of October 26, 2016: http://java.epa.gov/oppt_chemical_search/

Hazardous Substances Data Bank (HSDB)

10.8 General Manufacturing Information

Industry Processing Sectors

Food, beverage, and tobacco product manufacturing

EPA Chemicals under the TSCA

EPA TSCA Commercial Activity Status

Benzoic acid, 3,4,5-trihydroxy-, propyl ester: ACTIVE

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

EPA Chemicals under the TSCA

The Panel on Food Additives and Nutrient Sources added to Food (ANS), European Food Safety Authority (EFSA), concluded in a 2014 report, that the use of propyl gallate as food additive at the current uses and use levels is not of safety concern.

EFSA; Scientific Opinion on the re-evaluation of propyl gallate (E 310) as a food additive; ESFA Journal 12: 3642 (2014). Available from, as of Oct 24, 2016: http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2014.3642/pdf

Hazardous Substances Data Bank (HSDB)

Propyl gallate is used as an antioxidant in pesticide formulations at typical concentrations of 0.25% or less.

USEPA; Inert Reassessment Propyl Gallate (CAS Reg. No. 121-79-9), December 2005. Available from, as of Oct 24, 2016: https://www.epa.gov/sites/production/files/2015-04/documents/propyl.pdf

Hazardous Substances Data Bank (HSDB)

Used in foods restricted to 0.02% of fat content.

Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Rheinhold Co., 1993, p. 972

Hazardous Substances Data Bank (HSDB)

The antioxidant formulations most commonly used in edible products contain various combinations of BHA, BHT, and/or propyl gallate together with citric acid in suitable solvent.

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 202

Hazardous Substances Data Bank (HSDB)

Tocopherols, gum guaiac, and similar natural antioxidants usually lack potency in most products compared to combinations of BHA /butylated hydroxyanisole/, BHT /butylated hydroxytoluene/, and propyl gallate.

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 203

Hazardous Substances Data Bank (HSDB)

11 Identification

11.1 Analytic Laboratory Methods

A simple and fast luminescent method is used ... to resolve a mixture of two synthetic antioxidants, propyl gallate (PG) and butylated hydroxyanisole (BHA), by the joint use of the stopped-flow mixing technique and a T-format luminescence spectrometer. The determination of these compounds involves two different and independent reactions. On the one hand, PG determination is based on an energy transfer process that involves the formation of a lanthanide chelate with **terbium** in the presence of Triton **X-100** and **tri-n-octylphosphine oxide**. On the other hand, BHA is determined using a reaction between the oxidized form of **Nile Blue** and the antioxidant. Both systems are excited at the same excitation wavelength (310 nm), and the emission wavelengths are 545 and 665 nm for PG and BHA, respectively. The absence of overlap in the emission spectra makes it possible to measure separately the analytes in each channel of the instrument. Initial rate and equilibrium signal are used as analytical parameters and measured in 0.1 and 1 s for PG and BHA, respectively. Calibration graphs are linear over the range 0.09-3.5 ug/mL for PG and 0.3-15 ug/mL for BHA. The relative standard deviations of both systems are close to 2%. The proposed method is applied to the determination of these two antioxidants in several commercial food samples with recoveries ranging between 94.8 and 102.9% for PG and between 94.1 and 102.1% for BHA.

PMID:10691634

Aguilar-Caballos MP et al; J Agric Food Chem 48 (2): 312-7 (2000)

▸ **Hazardous Substances Data Bank (HSDB)**

An accurate and rapid method for simultaneous determination of antioxidants butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT) and propyl gallate (PG) in food by reversed-phase high performance liquid chromatography was established. The sample was extracted with **hexane**. Being filtrated and dried by N2, the residues in evaporator was dissolved in a certain amount of **water**-C2H5OH (1:4, V/V) and filtered with 0.5 micron of filter membrane for HPLC analysis. The chromatographic conditions were Radial-PAK C12 column, **methanol-water** (92:8, V/V) mobile phase adjusted to pH = 3 with **phosphoric acid** and UV-280 nm detector. By using external standard method the analytical results showed that the coefficients of variation of PG,BHA and BHT were 0.61, 0.08 and 1.44 respectively, linear correlation coefficients were more than 0.999 and recoveries were 92%-98% (n = 6). The lowest detection limit was 0.5 mg/L.

PMID:11327012

Li G et al; Se Pu 16 (3): 276-7 (1998)

▸ **Hazardous Substances Data Bank (HSDB)**

A flow-through optosensor with solid phase UV spectroscopic detection is proposed for the direct determination of single antioxidants, namely butylated hydroxyanisole (BHA) and n-propyl gallate (n-PG), without previous derivatization. The methods are based on the transient retention behavior of these compounds in a flow-through cell packed with C-18 silica using **ethanol-water** mixtures as a carrier, and on the intrinsic absorbance monitored at 290 and 283 nm, respectively. After recording the analytical signal, the antioxidants were easily and quickly desorbed from the solid support by the same carrier. For BHA, calibration graphs were linear over the range 1.0-300.0 mg/L using area as the analytical parameter. The relative standard deviation (RSD) was between 0.5 and 1.6%. For n-PG, calibration graphs were linear over the range 1.0-300.0 mg/L in area and the RSD was between 1.4 and 1.5%. The methods were applied to the determination of these antioxidants in several food and cosmetics samples, and were validated using the standard additions method and an HPLC reference method.

PMID:11445959

Capitan-Vallvey LF et al; Analyst 126 (6): 897-902 (2001)

▸ **Hazardous Substances Data Bank (HSDB)**

An HPLC method with fluorescence detection was developed for the determination of propyl gallate, **nordihydroguaiaretic acid**, butylated hydroxyanisole (2- and 3-tert-butyl-4-hydroxyanisole), **tert-butylhydroquinone** and **octyl gallate** in edible oils and foods. The antioxidants in edible oil were isolated directly with **acetonitrile** saturated with **n-hexane**. The antioxidants in food were extracted with **ethyl acetate** and the extract was concentrated under vacuum. They were isolated from the residue with **acetonitrile** saturated with **n-hexane**. The **acetonitrile** layer was centrifuged at 5,000 rpm for 10 min. The HPLC separation was performed on a Symmetry C18 column (3.5 microns, 4.6 mm i.d. x 150 mm) using a mixture of 5% **acetic acid-acetonitrile-methanol** (4:3:3, v/v/v) as the mobile phase and monitored by using a fluorescence detector with time programming. Sample peaks were identified by comparison of the fluorescence spectra with those of antioxidant standards. Average recoveries of fortified antioxidants at 100 micrograms/g were 72.1-99.6%. Coefficients of variation were 0.7-7.2%.

PMID:12092411

Oishi M et al; Shokuhin Eiseigaku Zasshi 43 (2): 104-9 (2002)

▸ **Hazardous Substances Data Bank (HSDB)**

For more Analytic Laboratory Methods (Complete) data for PROPYL GALLATE (12 total), please visit the **HSDB record page**.

▸ **Hazardous Substances Data Bank (HSDB)**

12 Safety and Hazards

12.1 Hazards Identification

12.1.1 GHS Classification

Showing 1 of 5 View More

Pictogram(s)	 Irritant
Signal	Warning
GHS Hazard Statements	H302: Harmful if swallowed [Warning Acute toxicity, oral] H317: May cause an allergic skin reaction [Warning Sensitization, Skin]
Precautionary Statement Codes	P261, P264, P270, P272, P280, P301+P312, P302+P352, P321, P330, P333+P313, P363, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

EU REGULATION (EC) No 1272/2008

12.1.2 Hazard Classes and Categories

Showing 2 of 4 View More

Acute Tox. 4 *

Skin Sens. 1

EU REGULATION (EC) No 1272/2008

Acute Tox. 4 (100%)

Skin Sens. 1 (99.95%)

European Chemicals Agency (ECHA)

12.1.3 Health Hazards

SYMPTOMS: Symptoms of exposure to this compound may include irritation of the skin, eyes, mucous membranes and upper respiratory tract. Other symptoms include gasping respirations and convulsions. Brief skin contact may dry the skin. Prolonged or repeated contact can cause dermatitis and sensitization of the skin. Aspiration into the lungs may cause chemical pneumonia. ACUTE/CHRONIC HAZARDS: This compound may be harmful by inhalation or ingestion. It is an irritant of the skin, eyes, mucous membranes and upper respiratory tract. When heated to decomposition it emits acrid smoke, irritating fumes and toxic fumes of carbon monoxide and carbon dioxide. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

12.1.4 Fire Hazards

This chemical is combustible. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

12.1.5 Fire Potential

Combustible when exposed to heat or flame ... .

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3084

Hazardous Substances Data Bank (HSDB)

12.1.6 Skin, Eye, and Respiratory Irritations

/LABORATORY ANIMALS: Acute Exposure/ Guinea pig: 10% /propyl gallate/ in propylene glycol applied to shaved skin for 48 hours /resulted in/ no local lesions or primary irritation. /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: https://www3.epa.gov/

Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ Rabbit: <1 percent /propyl gallate/ in a lipstick. Primary skin irritation test - applied to intact and abraded skin, three 24-hour applications. Not a primary irritant. /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: https://www3.epa.gov/

Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ Rabbit: Lipstick containing <7% propyl gallate. Nonirritant /to eyes/. /from table/

*EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 6 (2005). Available from, as of October 12, 2016: **https://www3.epa.gov/***

▸ Hazardous Substances Data Bank (HSDB)

12.2 First Aid Measures

12.2.1 First Aid

EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with **water** or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop. SKIN: IMMEDIATELY flood affected skin with **water** while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and **water**. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment. INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing. INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of **water** to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

▸ CAMEO Chemicals

12.3 Fire Fighting

Fires involving this material can be controlled with a dry chemical, **carbon dioxide** or **Halon** extinguisher. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

▸ CAMEO Chemicals

12.3.1 Fire Fighting Procedures

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

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

▸ Hazardous Substances Data Bank (HSDB)

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

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

▸ Hazardous Substances Data Bank (HSDB)

12.4 Accidental Release Measures

12.4.1 Cleanup Methods

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Environmental precautions: Do not let product enter drains. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

▸ Hazardous Substances Data Bank (HSDB)

12.4.2 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. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber; Contaminated packaging: Dispose of as unused product.

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

▸ Hazardous Substances Data Bank (HSDB)

12.4.3 Preventive Measures

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Environmental precautions: Do not let product enter drains.

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

▸ Hazardous Substances Data Bank (HSDB)

Precautions for safe handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed.

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

Hazardous Substances Data Bank (HSDB)

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

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **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 Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

Hazardous Substances Data Bank (HSDB)

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. Ensure that the local ventilation moves the contaminant away from the worker.

Hazardous Substances Data Bank (HSDB)

12.5 Handling and Storage

12.5.1 Nonfire Spill Response

SMALL SPILLS AND LEAKAGE: Should a spill occur while you are handling this chemical, FIRST REMOVE ALL SOURCES OF IGNITION, then you should dampen the solid spill material with 60-70% **ethanol** and transfer the dampened material to a suitable container. Use absorbent paper dampened with 60-70% **ethanol** to pick up any remaining material. Seal the absorbent paper, and any of your clothes, which may be contaminated, in a vapor-tight plastic bag for eventual disposal. Solvent wash all contaminated surfaces with 60-70% **ethanol** followed by washing with a soap and **water** solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned. STORAGE PRECAUTIONS: You should store this chemical under ambient temperatures, and keep it away from oxidizing materials. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

12.5.2 Storage Conditions

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

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

Hazardous Substances Data Bank (HSDB)

12.6 Exposure Control and Personal Protection

12.6.1 Allowable Tolerances

Residues of propyl gallate are exempted from the requirement of a tolerance when used as an antioxidant in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest.

*40 CFR 180.910 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: **http://www.ecfr.gov***

Hazardous Substances Data Bank (HSDB)

Residues of propyl gallate are exempted from the requirement of a tolerance when used as a antioxidant in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals.

*40 CFR 180.930 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: **http://www.ecfr.gov***

Hazardous Substances Data Bank (HSDB)

12.6.2 Personal Protective Equipment (PPE)

RECOMMENDED RESPIRATOR: Where the neat test chemical is weighed and diluted, wear a NIOSH-approved half face respirator equipped with an organic vapor/acid gas cartridge (specific for organic vapors, HCl, acid gas and SO2) with a dust/mist filter. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

CAMEO Chemicals

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

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

Hazardous Substances Data Bank (HSDB)

Skin protection: Handle with gloves.

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

Hazardous Substances Data Bank (HSDB)

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

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

Hazardous Substances Data Bank (HSDB)

Respiratory protection: For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

▸ Hazardous Substances Data Bank (HSDB)

12.7 Stability and Reactivity

12.7.1 Air and Water Reactions

Insoluble in water.

▸ CAMEO Chemicals

12.7.2 Reactive Group

Esters, Sulfate Esters, Phosphate Esters, Thiophosphate Esters, and Borate Esters

Phenols and Cresols

▸ CAMEO Chemicals

12.7.3 Reactivity Profile

PROPYL GALLATE can react with oxidizing agents. Incompatible with strong acids, strong bases and strong reducing agents. Darkens in the presence of iron and iron salts. Contact with metals should be avoided (NTP, 1992).

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

▸ CAMEO Chemicals

12.7.4 Hazardous Reactivities and Incompatibilities

Incompatible materials: Strong oxidizing agents, strong acids, strong bases, strong reducing agents

*Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: **http://www.sigmaaldrich.com/safety-center.html***

▸ Hazardous Substances Data Bank (HSDB)

Can react with oxidizing materials.

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3084

▸ Hazardous Substances Data Bank (HSDB)

12.8 Regulatory Information

12.8.1 FIFRA Requirements

Residues of propyl gallate are exempted from the requirement of a tolerance when used as an antioxidant in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops or to raw agricultural commodities after harvest.

*40 CFR 180.910 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: **http://www.ecfr.gov***

▸ Hazardous Substances Data Bank (HSDB)

Residues of propyl gallate are exempted from the requirement of a tolerance when used as a antioxidant in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals.

*40 CFR 180.930 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: **http://www.ecfr.gov***

▸ Hazardous Substances Data Bank (HSDB)

12.8.2 FDA Requirements

The food additive chewing gum base may be safely used in the manufacture of chewing gum in accordance with the following prescribed conditions: (a) The food additive consists of one or more of the following substances that meet the specifications and limitations prescribed in this paragraph, used in amounts not to exceed those required to produce the intended physical or other technical effect. Propyl gallate is included on this list. Not to exceed antioxidant content of 0.1% when used alone or in any combination.

*21 CFR 172.615 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 21, 2016: **http://www.ecfr.gov***

▸ Hazardous Substances Data Bank (HSDB)

Substances classified as antioxidants, when migrating from food-packaging material (limit of addition to food, 0.005 percent) shall include: propyl gallate.

*21 CFR 181.24 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 21, 2016: **http://www.ecfr.gov***

▸ Hazardous Substances Data Bank (HSDB)

Substance added directly to human food affirmed as generally recognized as safe (GRAS). ... Good manufacturing practice results in a maximum total content of antioxidants of 0.02 percent of the fat or oil content, including the essential (volatile) oil content, of the food.

*21 CFR 184.1660 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 21, 2016: **http://www.ecfr.gov***

▸ Hazardous Substances Data Bank (HSDB)

This substance is generally recognized as safe for use in food when the total content of antioxidants is not over 0.02 percent of fat or oil content, including essential (volatile) oil content of the food, provided the substance is used in accordance with good manufacturing or feeding practice.

21 CFR 582.3660 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 21, 2016: ***http://www.ecfr.gov***

- **Hazardous Substances Data Bank (HSDB)**

12.9 Other Safety Information

12.9.1 Toxic Combustion Products

Special hazards arising from the substance or mixture: Carbon oxides

Sigma-Aldrich; Safety Data Sheet for Propyl gallate. Product Number: P3130, Version 4.4 (Revision Date 06/28/2014). Available from, as of October 7, 2016: ***http://www.sigmaaldrich.com/safety-center.html***

- **Hazardous Substances Data Bank (HSDB)**

12.9.2 Special Reports

DHHS/NTP; Toxicology & Carcinogenesis Studies of Propyl Gallate in F344/N Rats and B6C3F1 Mice (Feed Study) Technical Report Series No. 240 (1982) NIH Publication No. 83-1796[Available from, as of October 10, 2016: https://ntp.niehs.nih.gov/]

- **Hazardous Substances Data Bank (HSDB)**

International Programme on Chemical Safety/World Health Organization; Food Additives Series 32, Gallates (1993)[Available from, as of October 10, 2016: http://www.inchem.org/documents/jecfa/jecmono/v32je02.htm]

- **Hazardous Substances Data Bank (HSDB)**

13 Toxicity

13.1 Toxicological Information

13.1.1 Acute Effects

ChemIDplus

13.1.2 Interactions

The antioxidant propyl gallate (PG) induced lipid peroxidation in combination with non-toxic Cu(II) concentrations in human fibroblasts. This was measured by the **thiobarbituric acid** assay (TBA assay) and by detection of accumulating fluorescent products after a 1-hr treatment of cells with CuCl2/PG at concentrations higher than 0.125 mM. PG alone led to a significant reduction of **thiobarbituric acid**-reactive substances (TBARS) demonstrating its antioxidative properties. Time course studies of lipid peroxidation by PG/Cu(II) showed that formation of TBARS was preceded by a lag phase of 60 min. Thereafter, the TBARS value increased rapidly for 1 hr and then reached a constant maximum or slightly decreased. The induction of lipid peroxidation by PG/Cu(II) is probably due to the formation of reactive species like reactive oxygen species (ROS), Cu(I) and semiquinone radicals which are able to participate in initiation and propagation of lipid peroxidation. Combination effects of PG/Cu(II) were demonstrated also on inhibition of membrane-bound **succinate** dehydrogenase. Cytosolic esterases were affected only slightly. The greater susceptibility of membrane-bound enzymes is in accordance with the lipid peroxidation-inducing effects of PG/Cu(II).

PMID:10597027
Jacobi H et al; Toxicol Lett 110 (3): 183-90 (1999)

Hazardous Substances Data Bank (HSDB)

We looked at the in vitro effect of an antioxidant, propyl gallate (PG), on the antifungal activity of **miconazole** sulphosalicylate, **econazole** sulphosalicylate and **ketoconazole** against 40 clinical isolates of Candida albicans. The combination of **imidazole** and PG gave MIC values 10-150 times lower than those of **imidazole** alone. The optimal conditions for this enhanced activity were pH 6.2-8.0 and a fungal cell concentration lower than 3 x 10(5) cells/mL. The mechanism of the interaction between **imidazole** and PG is not known but may be as a result of an effect of PG on the P-450 cytochrome. ...

PMID:11185418
Strippoli V et al; Int J Antimicrob Agents 16 (1): 73-6 (2000)

Hazardous Substances Data Bank (HSDB)

Partial protection against liver damage by single oral doses of 2.5 or 0.25 ml/kg of **chloroform** was provided by ip injection of 150 mg/kg bw of propyl gallate ... .

International Programme on Chemical Safety/World Health Organization; Food Additives Series 32, Gallates (1993). Available from, as of October 10, 2016: ***http://www.inchem.org/documents/jecfa/jecmono/v32je02.htm***

Hazardous Substances Data Bank (HSDB)

Pregnant New Zealand white rabbits (on gestation day 12) were injected sc with propyl gallate (362-900 mg/kg bw) and **hydroxyurea** (600-750 mg/kg bw). The materials were injected either simultaneously or mixed over periods of 45 min. The extent of amelioration of the teratogenic effects of **hydroxyurea** was dependent on the dose of propyl gallate. There was a significant linear decrease in both resorptions and specific malformations with increasing doses of propyl gallate ... .

International Programme on Chemical Safety/World Health Organization; Food Additives Series 32, Gallates (1993). Available from, as of October 10, 2016: ***http://www.inchem.org/documents/jecfa/jecmono/v32je02.htm***

Hazardous Substances Data Bank (HSDB)

For more Interactions (Complete) data for PROPYL GALLATE (22 total), please visit the **HSDB record page**.

Hazardous Substances Data Bank (HSDB)

13.1.3 Toxicity Summary

IDENTIFICATION AND USE: Propyl gallate is white to creamy-white crystalline powder. It is used as an antioxidant for foods and cosmetics; especially fats, oils, emulsions, and waxes. It is used in transformer oils and as a stabilizer for synthetic vitamin A. It is also used as experimental medication. HUMAN EXPOSURE AND TOXICITY: Statistically significant increase in propyl gallate-positive rates on patch testing over the last decade have been reported. Propyl gallate produced contact dermatitis in 5 of 10 patients. Patients applied 20% in 70% **ethyl alcohol** to forearm daily for 24 days. 5 patients complained of pruritus and erythema. Propyl gallate was investigated in vitro at concentration of 0.5, 5.0 and 50 ug/mL employing WI-38 human embryonic lung cells for anaphase abnormalities. Propyl gallate was not mutagenic. ANIMAL STUDIES: In a 4-week oral toxicity study, rats ingested 0%, 0.1%, 0.5%, or 2.5% propyl gallate in feed. In rats ingesting the highest dose, a decrease in weight gain of more than 10%, dirty tails, thickening of the stomach wall, necrosis, and ulceration of the stomach mucosa, a moderate to severe granulomatous inflammatory response in the submucosa and muscular wall of the stomach, anemia, hyperplastic tubuli in the outer medulla of the kidneys, and increased activity of several microsomal and cytoplasmic drug-metabolizing enzymes in the liver were observed. Increased activity of hepatic drug metabolizing enzymes was also noted in rats treated with 0.5% propyl gallate. No effects were noted in those ingesting 0.1%. Guinea pigs fed 0.02% propyl gallate in the diet for 14 months and dogs fed 0.01% for a year showed no signs of toxicity. Administration to rats of 2.5% propyl gallate in the diet caused maternal toxicity and slight retardation of fetal development, but no teratogenic effects. In dose levels up to 250 mg/kg/day, propyl gallate had no effects on organogenesis in rabbits. At a concentration of 0-0.1 mg/plate, propyl gallate was mutagenic in S. typhimurium strain TA102, in the presence, but not the absence, of metabolic activation. An intraperitoneal injection of 900 mg/kg propyl gallate caused a positive result in a mouse micronucleus test. Propyl gallate was found to be negative when tested for mutagenicity using the

Salmonella/microsome preincubation assay with 5 Salmonella typhimurium strains (TA1535, TA1537, TA97, TA98, and TA100) in the presence and absence of metabolic activation. ECOTOXICITY STUDIES: The toxic effects of propyl gallate on aquatic organisms were investigated, using five model systems from four trophic levels. The most sensitive system was the hepatoma fish cell line PLHC-1 according to total protein content, with an EC(50) of 10 uM and a NOAEL of 1 uM at 72 hours, followed by the immobilization of Daphnia magna, the inhibition of bioluminescence of Vibrio fischeri, the salmonid fish cell line RTG-2 and the inhibition of the growth of Chlorella vulgaris.

Hazardous Substances Data Bank (HSDB)

13.1.4 Antidote and Emergency Treatment

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

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. 276-7

Hazardous Substances Data Bank (HSDB)

Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer **oxygen** by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if necessary ... . 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 ... . Administer activated **charcoal** ... . Dilution may be contraindicated because it may increase absorption. Do not use emetics ... . Cover skin burns with dry, sterile dressings after decontamination ... . Maintain body temperature. /Phenols and Related Compounds/

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. 277

Hazardous Substances Data Bank (HSDB)

Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques with a bag-valve-mask device may be beneficial. Consider drug therapy for pulmonary edema ... . Monitor cardiac rhythm and treat arrhythmias if necessary ... . Start IV administration of D5W TKO. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Consider vasopressors if patient is hypotensive with a normal fluid volume. Watch for signs of fluid overload ... . Administer 1% solution **methylene blue** if patient is symptomatic with severe hypoxia, cyanosis, and cardiac compromise not responding to **oxygen**. DIRECT PHYSICIAN ORDER ONLY ... . Treat seizures with **diazepam** (**Valium**) or **lorazepam** (**Ativan**) ... . Use **proparacaine hydrochloride** to assist eye irrigation ... . /Phenols and Related Compounds/

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. 277

Hazardous Substances Data Bank (HSDB)

13.1.5 Human Toxicity Excerpts

/HUMAN EXPOSURE STUDIES/ ... The objectives were to assess the prevalence of allergic contact dermatitis to propyl gallate in our center from 1988 to 2005. From 1988 to 2005, 9529 patients were patch tested to the face series, 6973 were females and 2556 were males. Patch tests were read at 2 D and 4 D. Positive reactions were scored as per International Contact Dermatitis Research Group recommendations as negative, +, ++, and +++ reactions. Propyl gallate was used at a 1% petrolatum (pet.). A total of 55 patients had positive reactions to propyl gallate 1% pet. (0.57%), 46 were female (0.65%) and 9 were male (0.33%). Using chi-square, there was a significant difference ($p<0.05$) in the positivity rates between the 1988-96 period (0.45%) and the 1997-2005 period (0.77%). A review of our face series performed in the last 18 years has shown a statistically significant increase in propyl gallate-positive rates on patch testing over the last decade. An increase in its use in the cosmetic industry may well be the explanation for this. Nevertheless, a concomitant reduction of propyl gallate as an antioxidant in food, with oral tolerance being less likely to develop, may also be a contributing factor in the increasing trend of allergic contact dermatitis caused by propyl gallate.

PMID:18154559
Perez A et al; Contact Dermatitis 58 (1): 47-8 (2008)

Hazardous Substances Data Bank (HSDB)

/HUMAN EXPOSURE STUDIES/Propyl gallate produced contact dermatitis in 5 of 10 patients. Patients applied 20% in 70% **ethyl alc** to forearm daily for 24 days. 5 Patients complained of pruritus and erythema.

Kahn G et al; Arch Dermatol 109 (Apr): 506-9 (1974)

Hazardous Substances Data Bank (HSDB)

/CASE REPORTS/ A 29-year-old Turkish woman with allergic contact cheilitis from a lipstick was misdiagnosed as herpes labialis and subsequently worsened with the application of **Zovirax** cream. Patch tests were positive to **Zovirax** cream, **propylene glycol**, the patient's favorite lipstick and propyl gallate. No reaction was seen with **Zovirax** ophthalmic ointment and **Zovirax** tablet. The **propylene glycol** component of the **Zovirax** cream and the propyl gallate component of the lipstick were regarded as the responsible contact sensitizers. The differential diagnosis was challenging due to concomitant contact sensitization with these agents.

PMID:17680974
Ozkaya E et al; Australas J Dermatol 48 (3): 190-2 (2007)

Hazardous Substances Data Bank (HSDB)

/CASE REPORTS/ A 62-year-old man, with a 20-year history of seborrhoeic dermatitis, presented with a worsening of his dermatitis. He had previously been demonstrated to be allergic to various topical corticosteroids, so he had been using an emollient cream (Sebclair), containing **piroctone olamine** and various anti-inflammatory substances, for 6 months, with good effect. Patch testing to the cream and its ingredients revealed positive reactions to both propyl gallate and pentylene glycol. A positive reaction to **propylene glycol** was also detected, whereas patch testing to butylene glycol was negative. Complete remission followed avoidance of the offending substances.

PMID:20546226
Foti C et al; Australas J Dermatol 51 (2): 147-8 (2010)

Hazardous Substances Data Bank (HSDB)

For more Human Toxicity Excerpts (Complete) data for PROPYL GALLATE (20 total), please visit the **HSDB record page**.

Hazardous Substances Data Bank (HSDB)

13.1.6 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ Guinea pig: 10% /propyl gallate/ in **propylene glycol** applied to shaved skin for 48 hours /resulted in/ no local lesions or primary irritation. /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: ***https://www3.epa.gov/***

▸ **Hazardous Substances Data Bank (HSDB)**

/LABORATORY ANIMALS: Acute Exposure/ Rabbit: <1 percent /propyl gallate/ in a lipstick. Primary skin irritation test - applied to intact and abraded skin, three 24-hour applications. Not a primary irritant. /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: ***https://www3.epa.gov/***

▸ **Hazardous Substances Data Bank (HSDB)**

/LABORATORY ANIMALS: Acute Exposure/ Rabbit: 0.003 percent /propyl gallate/ in suntan cream. Primary skin irritation- intact and abraded, three 24-hour applications. No edema, not a primary skin irritant. /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: ***https://www3.epa.gov/***

▸ **Hazardous Substances Data Bank (HSDB)**

/LABORATORY ANIMALS: Acute Exposure/ Rabbit: 0.003 percent /propyl gallate/ in suntan oil. Primary skin irritation- intact, three 6-hour applications. Practically nonirritating. /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 6 (2005). Available from, as of October 12, 2016: ***https://www3.epa.gov/***

▸ **Hazardous Substances Data Bank (HSDB)**

For more Non-Human Toxicity Excerpts (Complete) data for PROPYL GALLATE (59 total), please visit the **HSDB record page**.

▸ **Hazardous Substances Data Bank (HSDB)**

13.1.7 Non-Human Toxicity Values

LD50 Rat oral 2100 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3084

▸ **Hazardous Substances Data Bank (HSDB)**

LD50 Mouse oral 1700 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3084

▸ **Hazardous Substances Data Bank (HSDB)**

LD50 Cat oral 400 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3084

▸ **Hazardous Substances Data Bank (HSDB)**

LD50 Pig oral > 2-6 g/kg bw /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: ***https://www3.epa.gov/***

▸ **Hazardous Substances Data Bank (HSDB)**

LD50 Rabbit oral 2.75 g/kg bw /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: ***https://www3.epa.gov/***

▸ **Hazardous Substances Data Bank (HSDB)**

LD50 Hamster oral 2.48 g/kg bw /from table/

EPA/Office of Prevention, Pesticides, and Toxic Substances; Memorandum: Reassessment of Two Exemptions from the Requirement of a Tolerance For Propyl Gallate (CAS Reg. No. 121-79-9) p. 5 (2005). Available from, as of October 12, 2016: ***https://www3.epa.gov/***

▸ **Hazardous Substances Data Bank (HSDB)**

LD50 Rat oral 3,600-3,800 mg/kg bw /From table/

International Programme on Chemical Safety/World Health Organization; Food Additives Series 32, Gallates (1993). Available from, as of October 10, 2016: ***http://www.inchem.org/documents/jecfa/jecmono/v32je02.htm***

▸ **Hazardous Substances Data Bank (HSDB)**

LD50 Mouse oral 2,000-3,000 mg/kg bw /From table/

International Programme on Chemical Safety/World Health Organization; Food Additives Series 32, Gallates (1993). Available from, as of October 10, 2016: ***http://www.inchem.org/documents/jecfa/jecmono/v32je02.htm***

▸ **Hazardous Substances Data Bank (HSDB)**

LD50 Rat ip 380 mg/kg bw /From table/

International Programme on Chemical Safety/World Health Organization; Food Additives Series 32, Gallates (1993). Available from, as of October 10, 2016: ***http://www.inchem.org/documents/jecfa/jecmono/v32je02.htm***

▸ **Hazardous Substances Data Bank (HSDB)**

13.1.8 Ecotoxicity Values

EC50; Species: Dreissena polymorpha (Zebra Mussel) shell length 5-8 mm; Conditions: freshwater, static, 17.0 °C (16.3-17.4 °C), pH 8.0 (7.3-8.7), hardness 146 mg/L CaCO3 (136-156 mg/L CaCO3), alkalinity 109 mg/L CaCO3 (98-120 mg/L CaCO3), dissolved **oxygen** 8.3 mg/L (6.0-11.2 mg/L); Concentration: 17800 ug/L for 48 hr (95% confidence interval: 11700-23800 ug/L); Effect: behavior, increased ability to detach from substrate /formulation/

Cope WG et al; Environ Toxicol Chem 16 (9): 1930-4 (1997) as cited in the ECOTOX database. Available from, as of October 5, 2016

▸ Hazardous Substances Data Bank (HSDB)

13.1.9 Ecotoxicity Excerpts

/AQUATIC SPECIES/ ... The toxic effects /of propyl gallate on aquatic organisms/ were investigated, using five model systems from four trophic levels. The most sensitive system was the hepatoma fish cell line PLHC-1 according to total protein content, with an EC(50) of 10 uM and a NOAEL of 1 uM at 72 hr, followed by the immobilization of Daphnia magna, the inhibition of bioluminescence of Vibrio fischeri, the salmonid fish cell line RTG-2 and the inhibition of the growth of Chlorella vulgaris. Although protein content, **neutral red** uptake, **methylthiazol** metabolization and acetylcholinesterase activity were reduced in PLHC-1 cells, stimulations were observed for lysosomal function, **succinate** dehydrogenase, **glucose-6-phosphate** dehydrogenase and **ethoxyresorufin**-O-deethylase activities. No changes were observed in metallothionein levels. The main morphological observations were the loss of cells and the induction of cell death mainly by necrosis but also by apoptosis. The protective and toxic effects of propyl gallate were evaluated. General antioxidants and **calcium** chelators did not modify the toxicity of propyl gallate, but an **iron**-dependent lipid peroxidation inhibitor gave 22% protection. The results also suggest that propyl gallate cytotoxicity is dependent on **glutathione** levels, which were modulated by malic acid diethyl ester and **2-oxothiazolidine-4-carboxylic acid**. According to the results, propyl gallate should be classified as toxic to aquatic organisms.

PMID:17382989
Zurita JL et al; Water Res 41 (12): 2599-611 (2007)

▸ Hazardous Substances Data Bank (HSDB)

13.1.10 Ongoing Test Status

EPA has released the Interactive Chemical Safety for Sustainability (iCSS) Dashboard. 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/[USEPA; ICSS Dashboard Application; Available from, as of September 8, 2016: http://actor.epa.gov/dashboard/]

▸ Hazardous Substances Data Bank (HSDB)

The following link will take the user to the National Toxicology Program (NTP) Test Agent Search Results page for propyl gallate, which tabulates all of the "Short-Term Toxicity Studies," "Long-term Carcinogenicity Studies," and "Genetic Toxicology Studies" performed with this chemical. Clicking on the "Testing Status" link will take the user to the status (i.e., in review, in progress, in preparation, on test, completed, etc.) and results of all the studies that the NTP has done on this chemical.[Available from: http://ntp.niehs.nih.gov/testing/status/agents/ts-10564-y.html]

▸ Hazardous Substances Data Bank (HSDB)

13.1.11 National Toxicology Program Studies

A carcinogenesis bioassay of propyl gallate was conducted by feeding diets containing 6,000 or 12,000 ppm propyl gallate to groups of 50 F344/N rats and 50 B6C3F1 mice of each sex for 103 wk. Groups of 50 untreated rats and 50 untreated mice of each sex served as controls. ... Under the conditions of this bioassay, propyl gallate was not considered to be carcinogenic for F344/N rats, although there was evidence of an incr proportion of low dose male rats with preputial gland tumors, islet cell tumors of the pancreas, and pheochromocytomas of the adrenal glands; rare tumors of the brain occurred in two low dose females. Propyl gallate was not considered to be carcinogenic for B6C3F1 mice of either sex, although the incr incidence of malignant lymphoma in male mice may have been related to dietary admin of propyl gallate.

DHHS/NTP; Toxicology & Carcinogenesis Studies of Propyl Gallate in F344/N Rats and B6C3F1 Mice (Feed Study) Technical Report Series No. 240 (1982) NIH Publication No. 83-1796. Available from, as of October 10, 2016: ***https://ntp.niehs.nih.gov/***

▸ Hazardous Substances Data Bank (HSDB)

13.2 Ecological Information

13.2.1 Environmental Fate/Exposure Summary

Propyl gallate's production and use as an antioxidant for cosmetics, foods, fats, oils, ethers, emulsifiers, waxes and transformer oils may result in its release to the environment through various waste streams. Propyl gallate's use as an antioxidant in pesticide formulations will result in its direct release to the environment. Propyl gallate has been detected in corn seed. If released to air, an estimated vapor pressure of 2.6X10-7 mm Hg at 25 °C indicates propyl gallate will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase propyl gallate will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 4.2 hours. Particulate-phase propyl gallate will be removed from the atmosphere by wet and dry deposition. Propyl gallate absorbs at wavelengths >290 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, propyl gallate is expected to have moderate mobility based upon an estimated Koc of 490. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 2.1X10-11 atm-cu m/mole. Propyl gallate is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Propyl gallate is reported to be biodegradable in the environment with ultimate aerobic degradation estimated to be weeks and primary degradation in days. If released into **water**, propyl gallate is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from **water** surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 7 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis half-lives of 12 and 1.2 years have been estimated at pH values of 7 and 8, respectively, at 25 °C. Photo-oxidation may have some importance in surface waters exposed to sunlight. Occupational exposure to propyl gallate may occur through inhalation and dermal contact with this compound at workplaces where propyl gallate is produced or used. Use data indicate that the general population may be exposed to propyl gallate via ingestion of food and dermal contact with consumer products containing propyl gallate. Propyl gallate is used as an antioxidant in a reported 167 cosmetic products. (SRC)

▸ Hazardous Substances Data Bank (HSDB)

13.2.2 Natural Pollution Sources

Propyl gallate was detected, not quantified in corn kernels (Zea mays, Poceae)(1).

(1) US Dept Agric; US Dept Agric, Agric Res Service. 1992-2016. Dr. Duke's Phytochemical and Ethnobotanical Databases. n-Propyl Gallate. Available from, as of Oct 25, 2016: ***https://phytochem.nal.usda.gov/phytochem/search***

▸ Hazardous Substances Data Bank (HSDB)

13.2.3 Artificial Pollution Sources

Propyl gallate's production and use as an antioxidant for cosmetics, foods, fats, oils, ethers, emulsifiers, waxes and transformer oils(1) may result in its release to the environment through various waste streams(SRC). Propyl gallate's use as an antioxidant in pesticide formulations, with typical concentrations of 0.25% or less(2), will result in its direct release to the environment(SRC).

(1) O'Neil MJ, ed; The Merck Index. 15th ed., Cambridge, UK: Royal Society of Chemistry, p. 1455 (2013) (2) USEPA; Inert Reassessment Propyl Gallate (CAS Reg. No. 121-79-9), December 2005. Available from, as of Oct 24, 2016: https://www.epa.gov/sites/production/files/2015-04/documents/propyl.pdf

Hazardous Substances Data Bank (HSDB)

13.2.4 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 490(SRC), determined from a structure estimation method(2), indicates that propyl gallate is expected to have moderate mobility in soil(SRC). Volatilization of propyl gallate from moist soil surfaces is not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 2.1X10-11 atm-cu m/mole(SRC), derived from its estimated vapor pressure, 2.6X10-7 mm Hg(2), and water solubility, 3490 mg/L(3). Propyl gallate is not expected to volatilize from dry soil surfaces(SRC) based upon its estimated vapor pressure(2). Propyl gallate is reported to be biodegradable in the environment(4) with ultimate aerobic degradation estimated to be weeks and primary degradation in days(5).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: http://www2.epa.gov/tsca-screening-tools (3) Yalkowsky SH et al; Handbook of Aqueous Solubility Data 2nd ed., Boca Raton, FL: CRC Press, p. 690 (2010) (4) Quinchia LA et al; J Agric Food Chem 59: 12917-12924 (2011) (5) USEPA; Inert Reassessment Propyl Gallate (CAS Reg. No. 121-79-9), December 2005. Available from, as of Oct 24, 2016: https://www.epa.gov/sites/production/files/2015-04/documents/propyl.pdf

Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 490(SRC), determined from a structure estimation method(2), indicates that propyl gallate is expected to adsorb moderately to suspended solids and sediment(SRC). Volatilization from water surfaces is not expected(3) based upon an estimated Henry's Law constant of 2.1X10-11 atm-cu m/mole(SRC) derived from its estimated vapor pressure, 2.6X10-7 mm Hg(2), and water solubility, 3490 mg/L(4). According to a classification scheme(5), an estimated BCF of 7(SRC), from its log Kow of 1.80(6) and a regression-derived equation(2), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Propyl gallate is reported to be biodegradable in the environment(7) with ultimate aerobic degradation estimated to be weeks and primary degradation in days(8). A base-catalyzed second-order hydrolysis rate constant of 0.018 L/mole-sec(SRC) was estimated using a structure estimation method(2); this corresponds to half-lives of 12 and 1.2 years at pH values of 7 and 8, respectively(2). Propyl gallate is reported to react readily with photo-oxidant radicals in aqueous media(9); therefore, photo-oxidation may have some importance in surface waters exposed to sunlight(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: http://www2.epa.gov/tsca-screening-tools (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (4) Yalkowsky SH et al; Handbook of Aqueous Solubility Data 2nd ed., Boca Raton, FL: CRC Press, p. 690 (2010) (5) Franke C et al; Chemosphere 29: 1501-14 (1994) (6) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 73 (1995) (7) Quinchia LA et al; J Agric Food Chem 59: 12917-12924 (2011) (8) USEPA; Inert Reassessment Propyl Gallate (CAS Reg. No. 121-79-9), December 2005. Available from, as of Oct 24, 2016: https://www.epa.gov/sites/production/files/2015-04/documents/propyl.pdf (9) Medina ME et al; Phys Chem Chem Phys 15: 13137-13146 (2013)

Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), propyl gallate, which has an estimated vapor pressure of 2.6X10-7 mm Hg at 25 °C(SRC), determined from a fragment constant method(2), will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase propyl gallate is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be 4.2 hours(SRC), calculated from its rate constant of 9.2X10-11 cu cm/molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(2). Particulate-phase propyl gallate may be removed from the air by wet and dry deposition(SRC). Propyl gallate absorbs at wavelengths >290 nm(3) and, therefore, may be susceptible to direct photolysis by sunlight(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 Oct 24, 2016: http://www2.epa.gov/tsca-screening-tools (3) Szymula M; J Cosmet Sci 55: 281-289 (2004). Available from, as of Oct 24, 2016: http://journal.scconline.org/pdf/cc2004/cc055n03/p00281-p00289.pdf

Hazardous Substances Data Bank (HSDB)

13.2.5 Environmental Biodegradation

AEROBIC: Propyl gallate is reported to be a biodegradable antioxidant effective in oxidatively stabilizing vegetable oils according to REACH (Registration, Evaluation, Authorization and Restriction of Chemicals) biodegradability regulations(1). Propyl gallate is expected to biodegrade in the environment with ultimate aerobic degradation estimated to be weeks and primary degradation in days(2).

(1) Quinchia LA et al; J Agric Food Chem 59: 12917-12924 (2011) (2) USEPA; Inert Reassessment Propyl Gallate (CAS Reg. No. 121-79-9), December 2005. Available from, as of Oct 24, 2016: https://www.epa.gov/sites/production/files/2015-04/documents/propyl.pdf

Hazardous Substances Data Bank (HSDB)

13.2.6 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of propyl gallate with photochemically-produced hydroxyl radicals has been estimated as 9.2X10-11 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 4.2 hours at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). A base-catalyzed second-order hydrolysis rate constant of 0.018 L/mole-sec(SRC) was estimated using a structure estimation method(1); this corresponds to half-lives of 12 and 1.2 years at pH values of 7 and 8, respectively(1). The UV spectrum of propyl gallate in water has two characteristic bands: maximum #1 at 217 nm and maximum #2 at 274 nm with decreasing absorbance extending to nearly 330 nm(2); therefore, propyl gallate may be susceptible to direct photolysis by sunlight(SRC). Propyl gallate is reported to react readily with photo-oxidant radicals in aqueous media(3); therefore, photo-oxidation may have some importance in surface waters exposed to sunlight(SRC). With respect to reaction fate in foods, it is reported that propyl gallate is stable in neutral or slightly acidic chemical environments but unstable when heated or in mild alkaline environment(4).

(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: http://www2.epa.gov/tsca-screening-tools (2) Szymula M; J Cosmet Sci 55: 281-289 (2004). Available from, as of Oct 24, 2016: http://journal.scconline.org/pdf/cc2004/cc055n03/p00281-p00289.pdf (3) Medina ME et al; Phys Chem Chem Phys 15: 13137-13146 (2013) (4) EFSA; Scientific Opinion on the re-evaluation of propyl gallate (E 310) as a food additive; ESFA Journal 12: 3642 (2014). Available from, as of Oct 24, 2016: http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2014.3642/pdf

Hazardous Substances Data Bank (HSDB)

13.2.7 Environmental Bioconcentration

An estimated BCF of 7 was calculated in fish for propyl gallate(SRC), using a log Kow of 1.80(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) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 73 (1995) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: http://www2.epa.gov/tsca-screening-tools (3) Franke C et al; Chemosphere 29: 1501-14 (1994)

Hazardous Substances Data Bank (HSDB)

13.2.8 Soil Adsorption/Mobility

Using a structure estimation method based on molecular connectivity indices(1), the Koc of propyl gallate can be estimated to be 490(SRC). According to a classification scheme(2), this estimated Koc value suggests that propyl gallate is expected to have moderate mobility in soil.

*(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: **http://www2.epa.gov/tsca-screening-tools** (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) Shahidi F, ed; Handbook of Antioxidants for Food Preservation. Waltham, MA; Woodhead Publishing, p. 54 (2015)*

▸ Hazardous Substances Data Bank (HSDB)

13.2.9 Volatilization from Water/Soil

The Henry's Law constant for propyl gallate is estimated as 2.1X10-11 atm-cu m/mole(SRC) derived from its estimated vapor pressure, 2.6X10-7 mm Hg(1), and water solubility, 3490 mg/L(2). This Henry's Law constant indicates that propyl gallate is expected to be essentially nonvolatile from water surfaces(3). Propyl gallate's estimated Henry's Law constant indicates that volatilization from moist soil surfaces is not expected to occur(SRC). Propyl gallate is not expected to volatilize from dry soil surfaces based upon its vapor pressure(SRC).

*(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Oct 24, 2016: **http://www2.epa.gov/tsca-screening-tools** (2) Yalkowsky SH et al; Handbook of Aqueous Solubility Data 2nd ed., Boca Raton, FL: CRC Press, p. 690 (2010) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)*

▸ Hazardous Substances Data Bank (HSDB)

13.2.10 Plant Concentrations

Propyl gallate was detected, not quantified in corn kernels (Zea mays, Poceae)(1).

*(1) US Dept Agric; US Dept Agric, Agric Res Service. 1992-2016. Dr. Duke's Phytochemical and Ethnobotanical Databases. n-Propyl Gallate. Available from, as of Oct 25, 2016: **https://phytochem.nal.usda.gov/phytochem/search***

▸ Hazardous Substances Data Bank (HSDB)

13.2.11 Probable Routes of Human Exposure

According to the 2012 TSCA Inventory Update Reporting data, 1 reporting facility estimates the number of persons reasonably likely to be exposed during the manufacturing, processing, or use of propyl gallate in the United States may be as low as 10-24 workers and as high as 10-24 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 Oct 21, 2016: **https://java.epa.gov/oppt_chemical_search/***

▸ Hazardous Substances Data Bank (HSDB)

Occupational exposure to propyl gallate may occur through inhalation and dermal contact with this compound at workplaces where propyl gallate is produced or used. Use data indicate that the general population may be exposed to propyl gallate via ingestion of food and dermal contact with consumer products containing propyl gallate(SRC). Propyl gallate is used as an antioxidant in a reported 167 cosmetic products, with a maximum concentration of 0.1%(1).

*(1) American College of Toxicology; International Journal of Toxicology (May 2007) 26: 89-118 (2007). Available from, as of Oct 24, 2016: **http://ijt.sagepub.com/content/26/3_suppl/89***

▸ Hazardous Substances Data Bank (HSDB)

13.2.12 Average Daily Intake

Average daily intake assessment: 0.25 - 1.11 mg/kg bw/day in adults(1). Propyl gallate has an ADI of 0-1.4 mg/kg bw/day established by the Joint FAO/WHO Expert Committee on Food Additives(JECFA)(2).

*(1) EFSA; Scientific Opinion on the re-evaluation of propyl gallate (E 310) as a food additive; ESFA Journal 12: 3642 (2014). Available from, as of Oct 24, 2016: **http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2014.3642/pdf***
*(2) USEPA; Inert Reassessment Propyl Gallate (CAS Reg. No. 121-79-9), December 2005. Available from, as of Oct 24, 2016: **https://www.epa.gov/sites/production/files/2015-04/documents/propyl.pdf***

▸ Hazardous Substances Data Bank (HSDB)

14 Associated Disorders and Diseases

- Comparative Toxicogenomics Database (CTD)

15 Literature

15.1 NLM Curated PubMed Citations

PubChem

15.2 Springer Nature References

Springer Nature

15.3 Thieme References

Thieme Chemistry

15.4 Wiley References

Wiley

15.5 Depositor Provided PubMed Citations

PubChem

15.6 Metabolite References

Human Metabolome Database (HMDB)

15.7 Chemical Co-Occurrences in Literature

PubChem

15.8 Chemical-Gene Co-Occurrences in Literature

PubChem

15.9 Chemical-Disease Co-Occurrences in Literature

PubChem

16 Patents

16.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

16.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

PATENTSCOPE (WIPO)

17 Biomolecular Interactions and Pathways

17.1 Drug-Gene Interactions

Drug Gene Interaction database (DGIdb)

17.2 Chemical-Gene Interactions

17.2.1 CTD Chemical-Gene Interactions

Comparative Toxicogenomics Database (CTD)

17.3 DrugBank Interactions

DrugBank

18 Biological Test Results

18.1 BioAssay Results

PubChem

19 Classification

19.1 Ontologies

19.1.1 MeSH Tree

MeSH

19.1.2 ChEBI Ontology

ChEBI

19.1.3 KEGG: Additive

KEGG

19.1.4 ChemIDplus

ChemIDplus

19.1.5 CAMEO Chemicals

CAMEO Chemicals

19.1.6 ChEMBL Target Tree

ChEMBL

19.1.7 UN GHS Classification

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

19.1.8 EPA CPDat Classification

- EPA Chemical and Products Database (CPDat)

19.1.9 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

20 Information Sources

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   https://cameochemicals.noaa.gov/chemical/20963

   CAMEO Chemical Reactivity Classification
   https://cameochemicals.noaa.gov/browse/react

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   Propyl gallate [NF]
   https://chem.nlm.nih.gov/chemidplus/sid/0000121799

   ChemIDplus Chemical Information Classification
   https://chem.nlm.nih.gov/chemidplus/

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   Propyl Gallate
   http://www.drugbank.ca/drugs/DB12450

4. **DTP/NCI**

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   propyl gallate
   https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=2626

5. **EPA Chemicals under the TSCA**

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   https://www.epa.gov/chemicals-under-tsca

6. **EPA DSSTox**

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   Propyl gallate
   https://comptox.epa.gov/dashboard/DTXSID5021201

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

   Propyl 3,4,5-trihydroxybenzoate
   https://echa.europa.eu/substance-information/-/substanceinfo/100.004.090

   Propyl 3,4,5-trihydroxybenzoate
   https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/72733

8. **Hazardous Substances Data Bank (HSDB)**

   PROPYL GALLATE
   https://pubchem.ncbi.nlm.nih.gov/source/hsdb/591

9. **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

   Propyl gallate
   http://www.hmdb.ca/metabolites/HMDB0033835

10. **EU Food Improvement Agents**

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

11. **ChEBI**

    N-propyl gallate
    http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:10607

    ChEBI Ontology
    http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

12. **FooDB**

    LICENSE

Propyl gallate
https://foodb.ca/compounds/FDB012003

13. ## Comparative Toxicogenomics Database (CTD)

http://ctdbase.org/detail.go?type=chem&acc=D011435

14. ## Drug Gene Interaction database (DGIdb)

https://www.dgidb.org/drugs/PROPYL GALLATE

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

propyl 3,4,5-trihydroxybenzoate
https://comptox.epa.gov/dashboard/DTXSID5021201#exposure
EPA CPDat Classification
https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

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

PROPYL GALLATE
https://apps.who.int/food-additives-contaminants-jecfa-database/chemical.aspx?chemID=1272

17. ## NORMAN Suspect List Exchange

NORMAN Suspect List Exchange Classification
https://www.norman-network.com/nds/SLE/

18. ## EU REGULATION (EC) No 1272/2008

propyl 3,4,5-trihydroxybenzoate
https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A32008R1272

19. ## Hazardous Chemical Information System (HCIS), Safe Work Australia

propyl 3,4,5-trihydroxybenzoate
http://hcis.safeworkaustralia.gov.au/HazardousChemical/Details?chemicalID=3699

20. ## NITE-CMC

Propyl 3,4,5-trihydroxybenzoate - FY2011
https://www.nite.go.jp/chem/english/ghs/11-mhlw-0077e.html

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

PROPYL GALLATE
https://www.cfsanappsexternal.fda.gov/scripts/fdcc/index.cfm?set=FoodSubstances&id=PROPYLGALLATE

22. ## FDA/SPL Indexing Data

8D4SNN7V92
https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

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

PROPYL GALLATE
https://www.femaflavor.org/flavor-library/propyl-gallate

24. ## NMRShiftDB

https://pubchem.ncbi.nlm.nih.gov/substance/8001833

25. ## MassBank of North America (MoNA)

Propyl gallate
http://mona.fiehnlab.ucdavis.edu/spectra/browse?inchikey=ZTHYODDOHIVTJV-UHFFFAOYSA-N

26. ## NIST Mass Spectrometry Data Center

Propyl gallate
http://www.nist.gov/srd/nist1a.cfm

27. ## SpectraBase

https://spectrabase.com/spectrum/DiN9wVI3XwG
https://spectrabase.com/spectrum/HjTOCVGALSz
https://spectrabase.com/spectrum/KQ2ll7ZwItV
https://spectrabase.com/spectrum/Bqcak4V97hi

https://spectrabase.com/spectrum/2ExSo0Uhg3K
https://spectrabase.com/spectrum/GOOqObhOTUB
https://spectrabase.com/spectrum/3Qxl0QAhmiV
https://spectrabase.com/spectrum/D5ZjnhoBjB1
https://spectrabase.com/spectrum/KuODVBXHibB
https://spectrabase.com/spectrum/Cxd9yujwddW
https://spectrabase.com/spectrum/HW18wHgo8Yv
https://spectrabase.com/spectrum/GQkJJ86IvEc
https://spectrabase.com/spectrum/6Rtpm0lnKqK
https://spectrabase.com/spectrum/LVw2b0SxXir
https://spectrabase.com/spectrum/8NeEslHfeDl

28. Springer Nature

29. Thieme Chemistry

30. Wikipedia

propyl gallate
https://en.wikipedia.org/wiki/Propyl_gallate

31. Wiley
https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=62643

32. MeSH

Propyl Gallate
https://www.ncbi.nlm.nih.gov/mesh/68011435

MeSH Tree
http://www.nlm.nih.gov/mesh/meshhome.html

Antioxidants
https://www.ncbi.nlm.nih.gov/mesh/68000975

33. PubChem
https://pubchem.ncbi.nlm.nih.gov

34. KEGG

Pharmaceutical additives in Japan
http://www.genome.jp/kegg-bin/get_htext?br08316.keg

35. 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

36. ChEMBL

Target Tree
https://www.ebi.ac.uk/chembl/target/browser

37. PATENTSCOPE (WIPO)

SID 403383845
https://pubchem.ncbi.nlm.nih.gov/substance/403383845