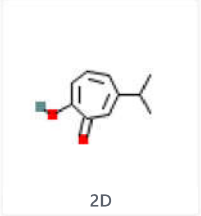
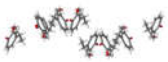
PubChem

COMPOUND SUMMARY

Hinokitiol

PubChem CID:	3611
Structure:	 2D  3D  Crystal Find Similar Structures
Chemical Safety:	 Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula:	$C_{10}H_{12}O_2$
Synonyms:	hinokitiol beta-Thujaplicin 499-44-5 4-Isopropyltropolone Hinokitol More...
Molecular Weight:	164.2 g/mol
Dates:	Modify: 2020-04-04 Create: 2005-03-25

Beta-thujaplicin is a monoterpenoid that is cyclohepta-2,4,6-trien-1-one substituted by a hydroxy group at position 2 and an isopropyl group at position 4. Isolated from Thuja plicata and Chamaecyparis obtusa, it exhibits antimicrobial activities. It has a role as an antifungal agent, an antibacterial agent, an antiplasmodial drug, an antineoplastic agent and a plant metabolite. It is an enol, a cyclic ketone and a monoterpenoid. It derives from a hydride of a cyclohepta-1,3,5-triene.

▸ ChEBI

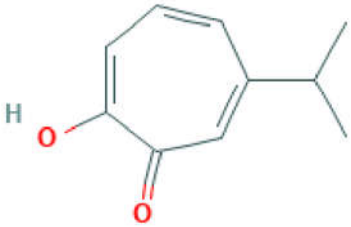
beta-Thujaplicin is found in fruits. beta-Thujaplicin occurs in Juniperus communis (juniper.

▸ Human Metabolome Database (HMDB)

1 Structures

1.1 2D Structure

Chemical Structure Depiction

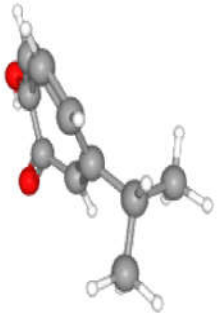


PubChem

1.2 3D Conformer

Interactive Chemical Structure Model

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



PubChem

1.3 Crystal Structures

CCDC Number	150506
Crystal Structure Data	DOI:10.5517/cc51m1v
Crystal Structure Depiction	

Associated Article	DOI:10.1016/S0040-4039(00)02133-X

The Cambridge Structural Database

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

2-hydroxy-6-propan-2-ylcyclohepta-2,4,6-trien-1-one

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

PubChem

2.1.2 InChI

InChI=1S/C10H12O2/c1-7(2)8-4-3-5-9(11)10(12)6-8/h3-7H,1-2H3,(H,11,12)

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

2.1.3 InChI Key

FUWUEFKEXZQKKA-UHFFFAOYSA-N

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

2.1.4 Canonical SMILES

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

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

PubChem

2.2 Molecular Formula

$C_{10}H_{12}O_2$

Wikipedia; PubChem

2.3 Other Identifiers

2.3.1 CAS

499-44-5

ChemIDplus; DTP/NCI; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA); Human Metabolome Database (HMDB)

2.3.2 Deprecated CAS

772-41-8, 333760-35-3, 1411673-73-8

ChemIDplus

2.3.3 European Community (EC) Number

207-880-7

European Chemicals Agency (ECHA)

2.3.4 NSC Number

18804

DTP/NCI

2.3.5 UNII

U5335D6EBI

FDA/SPL Indexing Data

2.3.6 DSSTox Substance ID

DTXSID6043911

EPA DSSTox

2.3.7 Wikipedia

Hinokitiol

Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

2-hydroxy-4-isopropyl- 2,4,6-cycloheptatriene-1-one
4-isopropyltropolone
beta-thujaplicin
beta-thujaplicin, sodium salt
hinokitiol

MeSH

2.4.2 Depositor-Supplied Synonyms

hinokitiol	beta-Isopropyltropolone	MLS001048906
beta-Thujaplicin	.beta.-Isopropyltropolon	Hinokitiol 4-Isopro
499-44-5	UNII-U5335D6EBI	U5335D6EBI
4-Isopropyltropolone	NSC 18804	2-Hydroxy-4-(1-me
Hinokitol	.beta.-Thujaplicine	CHEBI:10447
beta-Thujaplicine	2-hydroxy-4-(propan-2-yl)cyclohepta-2,4,6-trien-1-one	FUWUEFKEXZQKK
THUJAPLICIN, BETA	NSC18804	2-hydroxy-4-isopro
Tropolone, 4-isopropyl-	EINECS 207-880-7	SMR000387099
2-Hydroxy-4-isopropyl-2,4,6-cycloheptatrien-1-one	2-Hydroxy-4-isopropyl-2,4,6-cyclohepta-2,4,6-trien-1-one	2,4,6-CYCLOHEPTA
beta-Isopropyltropolon	2-Hydroxy-4-isopropylcyclohepta-2,4,6-trien-1-one	ss-Thujaplicine
Isopropyltropolone	BRN 2045206	b-Thujaplicin
2,4,6-Cycloheptatrien-1-one, 2-hydroxy-4-(1-methylethyl)-	CHEMBL48310	beta -thujaplicin
.beta.-Thujaplicin	AI3-28398	beta -thujaplicine

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	164.2 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
XLogP3-AA	2.1	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	2	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	1	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	164.08373 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Monoisotopic Mass	164.08373 g/mol	Computed by PubChem 2.1 (PubChem release 2019.06.18)
Topological Polar Surface Area	37.3 Å²	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	12	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	280	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

Solid

▶ Human Metabolome Database (HMDB)

3.2.2 Melting Point

52-52.5°C

▶ Human Metabolome Database (HMDB)

3.2.3 Solubility

1.2 mg/mL at 25 °C

▶ Human Metabolome Database (HMDB)

3.2.4 Octanol/Water Partition Coefficient

1.82 (LogP)

BIOBYTE STARLIST (2009)

EPA DSSTox

3.2.5 Kovats Retention Index

Standard non-polar	1559
Semi-standard non-polar	1559

NIST Mass Spectrometry Data Center

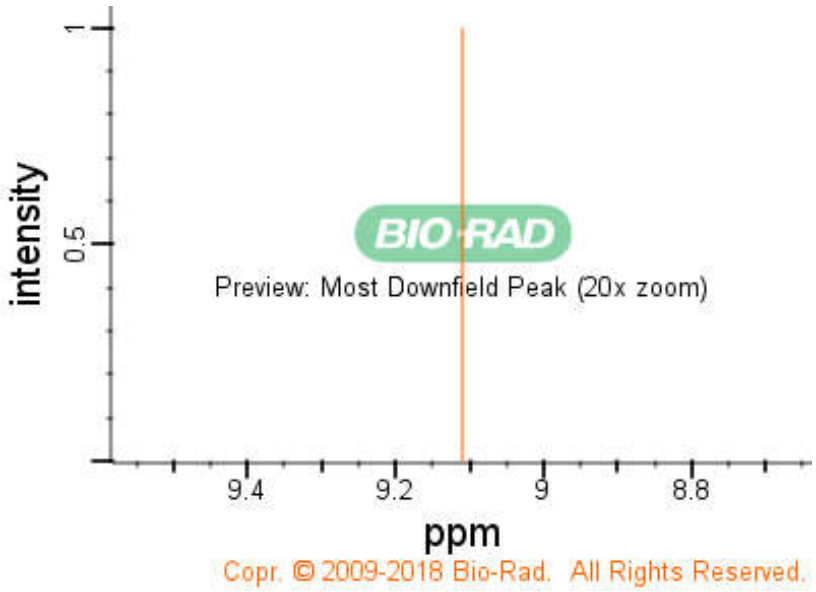
4 Spectral Information

4.1 1D NMR Spectra

1D NMR Spectra	NMRShiftDB Link

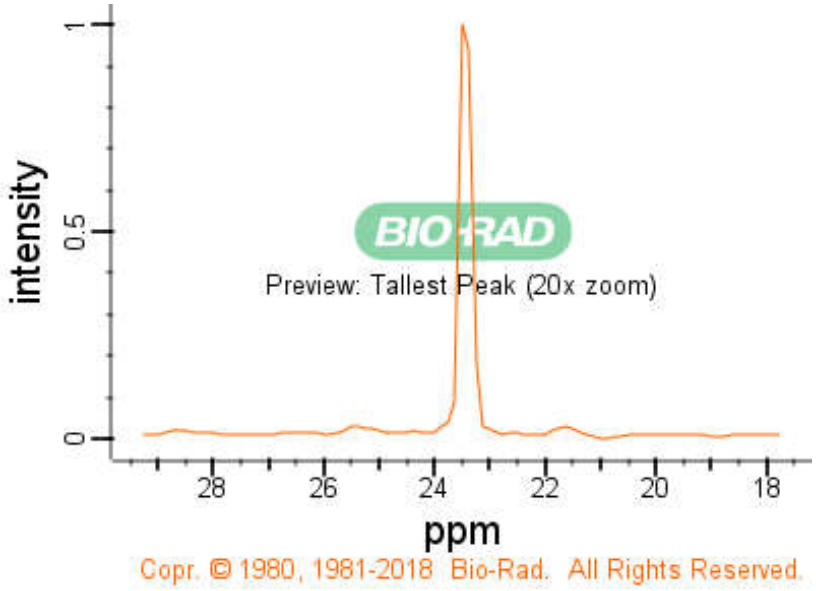
▶ NMRShiftDB

4.1.1 1H NMR Spectra

Instrument Name	Varian A-60
Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 2009-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

▶ SpectraBase

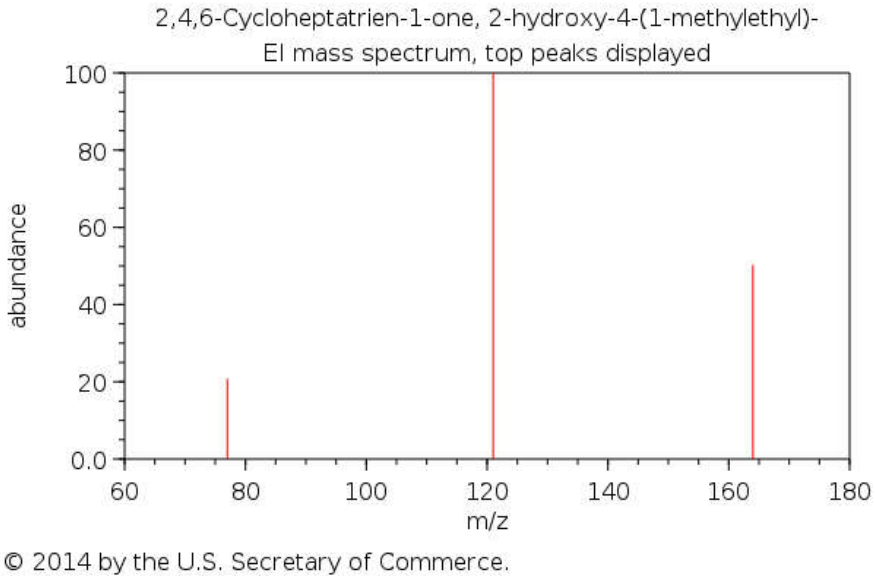
4.1.2 13C NMR Spectra

Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.2 Mass Spectrometry

4.2.1 GC-MS

NIST Number	292009
Library	Main library
Total Peaks	103
m/z Top Peak	121
m/z 2nd Highest	164
m/z 3rd Highest	77
Thumbnail	

NIST Mass Spectrometry Data Center

NIST Number	230996
Library	Replicate library
Total Peaks	97
m/z Top Peak	121
m/z 2nd Highest	164
m/z 3rd Highest	77
Thumbnail	

NIST Mass Spectrometry Data Center

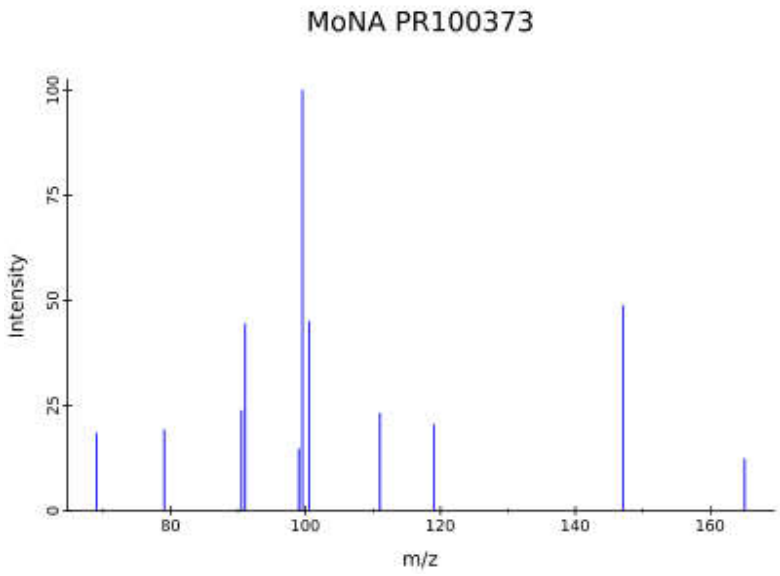
4.2.2 MS-MS

MS-MS	MS-MS Spectrum 439220 - beta-Thujaplicin (HMDB0035213) MS-MS Spectrum 439221 - beta-Thujaplicin (HMDB0035213) MS-MS Spectrum 448161 - beta-Thujaplicin (HMDB0035213)

Human Metabolome Database (HMDB)

4.2.3 LC-MS

Showing 2 of 5 View More

MoNA ID	PR100373
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2
Precursor Type	[M+H]+
precursor m/z	165.09153
Instrument	UPLC Q-Tof Premier, Waters
Instrument Type	LC-ESI-QTOF
Ionization	ESI
Ionization Mode	positive
Collision Energy	Ramp 5-60 V
Splash	splash10-0002-9600000000-60f1209a7a4a3d467962
Thumbnail	
Submitter	RIKEN Plant Science Center Team, Riken Plant Science Center

MassBank of North America (MoNA)

MoNA ID	PR100822
MS Category	Experimental
MS Type	LC-MS
MS Level	MS2

Precursor Type	[M-H]-
precursor m/z	163.07593
Instrument	UPLC Q-Tof Premier, Waters
Instrument Type	LC-ESI-QTOF
Ionization	ESI
Ionization Mode	negative
Collision Energy	Ramp 5-60 V
Splash	splash10-03di-0900000000-0a83b777d47c5cb70fe7
Thumbnail	
Submitter	RIKEN Plant Science Center Team, Riken Plant Science Center

MassBank of North America (MoNA)

4.2.4 Other MS

Showing 2 of 3 View More

MoNA ID	PS088001
MS Category	Experimental
MS Level	MS2
Precursor Type	[M+H]+
precursor m/z	165.18
Instrument	TQD, Waters
Instrument Type	Flow-injection QqQ/MS
Ionization	ESI
Ionization Mode	positive
Splash	splash10-014i-0900000000-03b8c846dad8f0abf40b
Thumbnail	

Submitter	ReSpect Consortium, RIKEN Center for Sustainable Resource Science

MassBank of North America (MoNA)

MoNA ID	PS088002
MS Category	Experimental
MS Level	MS2
Precursor Type	[M+H]+
precursor m/z	165.18
Instrument	TQD, Waters
Instrument Type	Flow-injection QqQ/MS
Ionization	ESI
Ionization Mode	positive
Splash	splash10-014i-0900000000-b6e9f10a223d9cb391b1
Thumbnail	
Submitter	ReSpect Consortium, RIKEN Center for Sustainable Resource Science

MassBank of North America (MoNA)

4.3 IR Spectra

4.3.1 FTIR Spectra

Technique	KBr WAFER
Source of Sample	Tokyo Kasei Kogyo Company, Ltd., Tokyo, Japan
Copyright	Copyright © 1980, 1981-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

Instrument Name	Bruker Tensor 27 FT-IR
Technique	KBr0
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	TCI Chemicals India Pvt. Ltd.
Catalog Number	H0142
Lot Number	MMKWF-BD
Copyright	Copyright © 2015-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.3.2 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	TCI Chemicals India Pvt. Ltd.
Catalog Number	H0142
Lot Number	MMKWF-BD
Copyright	Copyright © 2015-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.3.3 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

4.4 Raman Spectra

Instrument Name	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
Technique	FT-Raman
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	TCI Chemicals India Pvt. Ltd.
Catalog Number	H0142
Lot Number	MMKWF-BD
Copyright	Copyright © 2015-2018 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

PubChem

5.2 Related Compounds

Same Parent, Exact	23 Records
Mixtures, Components, and Neutralized Forms	27 Records
Similar Compounds	64 Records
Similar Conformers	2,338 Records

PubChem

5.3 Substances

5.3.1 Related Substances

All	227 Records
Same	156 Records
Mixture	71 Records

PubChem

5.3.2 Substances by Category

PubChem

5.4 Entrez Crosslinks

PubMed	55 Records
Taxonomy	1 Record
Gene	4 Records

PubChem

5.5 NCBI LinkOut

NCBI

6 Chemical Vendors

- PubChem

7 Pharmacology and Biochemistry

7.1 MeSH Pharmacological Classification

Antineoplastic Agents, Phytogenic

Agents obtained from higher plants that have demonstrable cytostatic or antineoplastic activity. (See all compounds classified as Antineoplastic Agents, Phytogenic.)

▶ MeSH

Iron Chelating Agents

Organic chemicals that form two or more coordination links with an iron ion. Once coordination has occurred, the complex formed is called a chelate. The iron-binding porphyrin group of hemoglobin is an example of a metal chelate found in biological systems. (See all compounds classified as Iron Chelating Agents.)

▶ MeSH

Anti-Infective Agents

Substances that prevent infectious agents or organisms from spreading or kill infectious agents in order to prevent the spread of infection. (See all compounds classified as Anti-Infective Agents.)

▶ MeSH

7.2 Human Metabolite Information

7.2.1 Metabolite Description

beta-Thujaplicin is found in fruits. beta-Thujaplicin occurs in Juniperus communis (juniper.

▶ Human Metabolome Database (HMDB)

7.2.2 Cellular Locations

Cytoplasm
Extracellular

▶ Human Metabolome Database (HMDB)

8 Use and Manufacturing

8.1 Uses

EPA CPDat Chemical and Product Categories

▶ EPA Chemical and Products Database (CPDat)

8.2 General Manufacturing Information

EPA TSCA Commercial Activity Status

2,4,6-Cycloheptatrien-1-one, 2-hydroxy-4-(1-methylethyl)-: ACTIVE

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

▶ EPA Chemicals under the TSCA

9 Safety and Hazards

9.1 Hazards Identification

9.1.1 GHS Classification

Pictogram(s)	 Irritant
Signal	Warning
GHS Hazard Statements	Aggregated GHS information provided by 167 companies from 2 notifications to the ECHA C&L Inventory. H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral] Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.
Precautionary Statement Codes	P264, P270, P301+P312, P330, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

▶ European Chemicals Agency (ECHA)

10 Toxicity

10.1 Toxicological Information

10.1.1 Acute Effects

- ChemIDplus

11 Literature

11.1 NLM Curated PubMed Citations

PubChem

11.2 Springer Nature References

Springer Nature

11.3 Thieme References

Thieme Chemistry

11.4 Depositor Provided PubMed Citations

PubChem

11.5 Metabolite References

Human Metabolome Database (HMDB)

11.6 Chemical Co-Occurrences in Literature

PubChem

11.7 Chemical-Gene Co-Occurrences in Literature

PubChem

11.8 Chemical-Disease Co-Occurrences in Literature

PubChem

12 Patents

12.1 Depositor-Supplied Patent Identifiers

PubChem

Link to all deposited patent identifiers

PubChem

12.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

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

PATENTSCOPE (WIPO)

13 Biological Test Results

13.1 BioAssay Results

PubChem

14 Classification

14.1 Ontologies

14.1.1 MeSH Tree

MeSH

14.1.2 ChEBI Ontology

ChEBI

14.1.3 KEGG: Phytochemical Compounds

KEGG

14.1.4 KEGG: Risk Category of Japanese OTC Drugs

KEGG

14.1.5 KEGG: OTC drugs

KEGG

14.1.6 WIPO IPC

WIPO

14.1.7 ChemIDplus

ChemIDplus

14.1.8 ChEMBL Target Tree

ChEMBL

14.1.9 UN GHS Classification

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

14.1.10 EPA CPDat Classification

EPA Chemical and Products Database (CPDat)

15 Information Sources

FILTER BY SOURCE: ALL SOURCES

1. ## ChEBI

Beta-thujaplicin
http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:10447

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

2. ## Human Metabolome Database (HMDB)

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http://www.hmdb.ca/citing

beta-Thujaplicin
http://www.hmdb.ca/metabolites/HMDB0035213

3. ## ChemIDplus

LICENSE

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

beta-Thujaplicin
https://chem.nlm.nih.gov/chemidplus/sid/0000499445

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

4. ## DTP/NCI

hinokitiol
https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=18804

5. ## EPA Chemicals under the TSCA

LICENSE

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

2,4,6-Cycloheptatrien-1-one, 2-hydroxy-4-(1-methylethyl)-
https://www.epa.gov/chemicals-under-tsca

6. ## EPA DSSTox

LICENSE

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

beta-Thujaplicin
https://comptox.epa.gov/dashboard/DTXSID6043911

7. ## European Chemicals Agency (ECHA)

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

2-hydroxy-4-isopropyl-2,4,6-cyclohepta-2,4,6-trien-1-one
https://echa.europa.eu/substance-information/-/substanceinfo/100.007.165

2-hydroxy-4-isopropyl-2,4,6-cyclohepta-2,4,6-trien-1-one
https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/53570

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

LICENSE

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

hinokitiol
https://comptox.epa.gov/dashboard/DTXSID6043911#exposure

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

9. FDA/SPL Indexing Data

U5335D6EBI
https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

10. MassBank of North America (MoNA)

Hinokitiol
http://mona.fiehnlab.ucdavis.edu/spectra/browse?inchikey=FUWUEFKEXZQKKA-UHFFFAOYSA-N

11. NIST Mass Spectrometry Data Center

2,4,6-Cycloheptatrien-1-one, 2-hydroxy-4-(1-methylethyl)-
http://www.nist.gov/srd/nist1a.cfm

12. NMRShiftDB

https://pubchem.ncbi.nlm.nih.gov/substance/87691382

13. SpectraBase

https://spectrabase.com/spectrum/KkebYVpOFTk
https://spectrabase.com/spectrum/6qgOI7eBc3z
https://spectrabase.com/spectrum/Hmq4gLKHPBQ
https://spectrabase.com/spectrum/3Jruu0UZjLL
https://spectrabase.com/spectrum/KYL0U2Gz5Eb
https://spectrabase.com/spectrum/HpO25o5ehba
https://spectrabase.com/spectrum/5zBfBQkLVy7

14. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/341145543
https://pubchem.ncbi.nlm.nih.gov/substance/341165269

15. The Cambridge Structural Database

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=150506

16. Thieme Chemistry

17. Wikipedia

hinokitiol
https://en.wikipedia.org/wiki/Hinokitiol

18. PubChem

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

19. MeSH

beta-thujaplicin
https://www.ncbi.nlm.nih.gov/mesh/67009479

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

Antineoplastic Agents, Phytogenic
https://www.ncbi.nlm.nih.gov/mesh/68000972

Iron Chelating Agents
https://www.ncbi.nlm.nih.gov/mesh/68007502

Anti-Infective Agents
https://www.ncbi.nlm.nih.gov/mesh/68000890

20. KEGG

Phytochemical compounds

http://www.genome.jp/kegg-bin/get_htext?br08003.keg

Risk category of Japanese OTC drugs
http://www.genome.jp/kegg-bin/get_htext?br08312.keg

Classification of Japanese OTC drugs
http://www.genome.jp/kegg-bin/get_htext?br08313.keg

21. ## WIPO

International Patent Classification
http://www.wipo.int/classifications/ipc/

22. ## 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

23. ## ChEMBL

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

24. ## PATENTSCOPE (WIPO)

SID 403422954
https://pubchem.ncbi.nlm.nih.gov/substance/403422954

25. ## NCBI

https://www.ncbi.nlm.nih.gov/projects/linkout