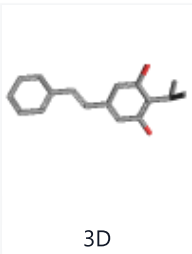
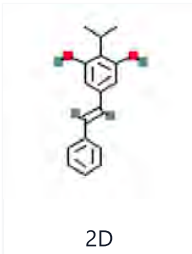


COMPOUND SUMMARY

Tapinarof

PubChem CID	6439522
Structure	 2D3D
Chemical Safety	 Environmental Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	C ₁₇ H ₁₈ O ₂
Synonyms	Benvitimod Tapinarof 79338-84-4 3,5-Dihydroxy-4-isopropylstilbene Vtama View More...
Molecular Weight	254.32 g/mol <i>Computed by PubChem 2.2 (PubChem release 2021.10.14)</i>
Dates	Create: 2006-04-28 Modify: 2024-11-30
Description	Benvitimod is a stilbenoid. ► ChEBI

Tapinarof is a novel, first-in-class, small-molecule AhR agonist that is indicated for the treatment of adult psoriasis. It is available as a topical cream to be applied to the affected area once daily. Tapinarof was first discovered as a metabolite (3,5-dihydroxy-4-isopropylstilbene) produced in *Photorhabdus luminescens*, a gram-negative bacillus that lives symbiotically with the *Heterorhabditis* nematodes. In 1959, it was noticed that *Heterorhabditis* with a high amount of 3,5-dihydroxy-4-isopropylstilbene did not putrefy once dead, thus suggesting its potential anti-inflammatory activity. Tapinarof received initial approval from the FDA in 2022.

► [DrugBank](#)

Tapinarof is an Aryl Hydrocarbon Receptor Agonist. The mechanism of action of tapinarof is as an Aryl Hydrocarbon Receptor Agonist.

► [FDA Pharm Classes](#)

[View More...](#)

Contents

Title and Summary	
1 Structures	▼
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3 Chemical and Physical Properties	▼
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5 Chemical Vendors	
6 Drug and Medication Information	▼
7 Pharmacology and Biochemistry	▼
8 Use and Manufacturing	▼
9 Safety and Hazards	▼

10 Toxicity



11 Associated Disorders and Diseases

12 Literature



13 Patents



14 Interactions and Pathways



15 Biological Test Results



16 Taxonomy

17 Classification

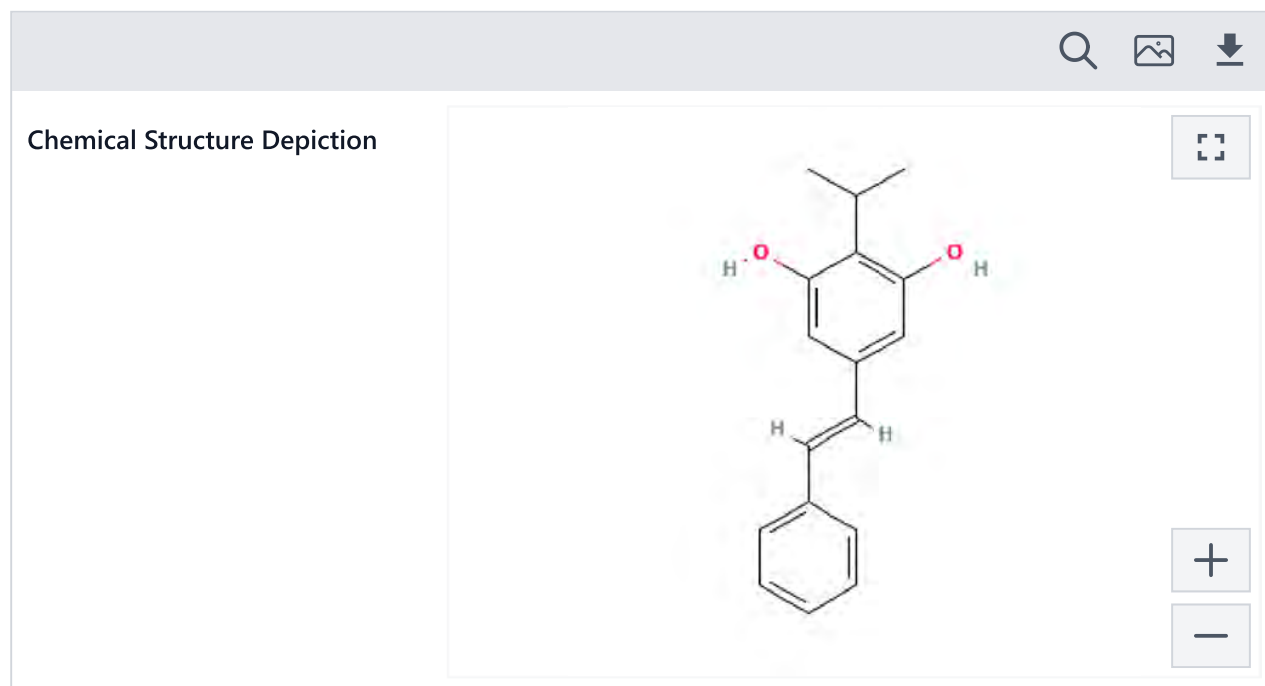


18 Information Sources

1 Structures



1.1 2D Structure



► PubChem

1.2 3D Conformer





► PubChem

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



5-[(E)-2-phenylethenyl]-2-propan-2-ylbenzene-1,3-diol

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

► PubChem

2.1.2 InChI



InChI=1S/C₁₇H₁₈O₂/c1-12(2)17-15(18)10-14(11-16(17)19)9-8-13-6-4-3-5-7-13/h3-12,18-19H,1-2H₃/b9-8+

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► PubChem

2.1.3 InChIKey



ZISJNXNHJRQYJO-CMDGGOBGSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.4 SMILES



CC(C)C1=C(C=C(C=C1O))/C=C/C2=CC=CC=C2)O

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

► [PubChem](#)

2.2 Molecular Formula



C₁₇H₁₈O₂

Computed by PubChem 2.2 (PubChem release 2021.10.14)

► [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



79338-84-4

► [CAS Common Chemistry](#); [ChemIDplus](#); [DrugBank](#); [EPA DSSTox](#); [European Chemicals Agency \(ECHA\)](#)

2.3.2 European Community (EC) Number



838-014-1

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

2.3.3 UNII



84HW7D0V04

► [FDA Global Substance Registration System \(GSRS\)](#)

2.3.4 ChEBI ID



CHEBI:215747

► ChEBI

2.3.5 ChEMBL ID



CHEMBL259571

► ChEMBL

2.3.6 DrugBank ID



DB06083

► DrugBank

2.3.7 DSSTox Substance ID



DTXSID301045262

► EPA DSSTox

2.3.8 KEGG ID



D11365

► KEGG

2.3.9 Metabolomics Workbench ID



99721

► Metabolomics Workbench

2.3.10 NCI Thesaurus Code



C152511

- ▶ NCI Thesaurus (NCIt)

2.3.11 Nikkaji Number



J478.929F

- ▶ Japan Chemical Substance Dictionary (Nikkaji)

J936.093J

- ▶ Japan Chemical Substance Dictionary (Nikkaji)

2.3.12 Pharos Ligand ID



CWFD8WKL4TMF

- ▶ Pharos

2.3.13 RXCUI



2602286

- ▶ NLM RxNorm Terminology

2.3.14 Wikidata



Q76386711

- ▶ Wikidata

2.3.15 Wikipedia



Tapinarof

- ▶ Wikipedia

2.4 Synonyms



2.4.1 MeSH Entry Terms



2-isopropyl-5-(2-phenylethenyl)benzene-1,3-diol
3,5-DH4IS
3,5-dihydroxy-4-isopropylstilbene
5-(2-phenylethenyl)-2-isopropyl-1,3-benzenediol
benvitimod
GSK2894512
tapinarof
WBI-1001

► Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms



Benvitimod	3,5-dihydroxy-4-isopropyl-trans-stilbene	1
Tapinarof	WBI 1001	1
79338-84-4	5-[(E)-2-phenylethenyl]-2-propan-2-ylbenzene-1,3-diol	1
3,5-Dihydroxy-4-isopropylstilbene	Tapinarof [USAN]	1
Vtama	UNII-84HW7D0V04	t
WBI-1001	2-Isopropyl-5-styrylbenzene-1,3-diol	5
GSK2894512	(E)-2-(1-Methylethyl)-5-(2-phenylethenyl)-1,3-benzenediol	5
3,5-DH4IS	115781-08-3	(
(E)-2-isopropyl-5-styrylbenzene-1,3-diol	84HW7D0V04	1
GSK-2894512	WB-1001	7

► PubChem

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference

Molecular Weight	254.32 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3-AA	4.6	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	254.130679813 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	254.130679813 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	40.5Å ²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	19	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	280	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
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	1	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 2021.10.14)

▶ [PubChem](#)

3.2 Chemical Classes



3.2.1 Drugs



3.2.1.1 Human Drugs



Breast Feeding; Lactation; Milk, Human; Dermatological Agents

▶ [Drugs and Lactation Database \(LactMed\)](#)

Human drug -> Prescription

▶ [Drugs@FDA](#)

Human drug -> Active ingredient (TAPINAROF)

▶ [Drugs@FDA](#)

3.2.2 Endocrine Disruptors



Potential endocrine disrupting compound

S109 | PARCEDC | List of 7074 potential endocrine disrupting compounds (EDCs) by PARC T4.2 | DOI:10.5281/zenodo.10944198

▶ [NORMAN Suspect List Exchange](#)

4 Related Records



4.1 Related Compounds with Annotation



Follow these links to [do a live 2D search](#) or [do a live 3D search](#) for this compound, sorted by annotation score. This section is deprecated (see [here](#) for details), but these live search links provide equivalent functionality to the table that was previously shown here.

▶ [PubChem](#)

4.2 Related Compounds



Same Connectivity Count	3
Same Parent, Connectivity Count	3
Mixtures, Components, and Neutralized Forms Count	8
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

▶ [PubChem](#)

4.3 Substances

?

↗

4.3.1 PubChem Reference Collection SID

?

↗

483927639

▶ [PubChem](#)

4.3.2 Related Substances

?

↗

All Count	120
Same Count	112
Mixture Count	8

▶ [PubChem](#)

4.3.3 Substances by Category

?

↗



▶ PubChem

4.4 Entrez Crosslinks



PubMed Count	7
Taxonomy Count	1
Gene Count	7

▶ PubChem

5 Chemical Vendors



▶ PubChem

6 Drug and Medication Information



6.1 Drug Indication



Tapinarof is indicated for the topical treatment of plaque psoriasis in adults.

▶ [DrugBank](#)



▶ [Open Targets](#)

6.2 Drug Classes



Breast Feeding; Lactation; Milk, Human; Dermatological Agents

▶ [Drugs and Lactation Database \(LactMed\)](#)

6.3 FDA Approved Drugs



▶ [Drugs@FDA](#)

6.4 FDA Orange Book



▶ [FDA Orange Book](#)

6.5 FDA National Drug Code Directory



▶ [National Drug Code \(NDC\) Directory](#)

6.6 Drug Labels



Drug and label



▶ [DailyMed](#)

Active ingredient and drug



▶ [DailyMed](#)

6.7 Clinical Trials

6.7.1 ClinicalTrials.gov



▶ [ClinicalTrials.gov](#)

7 Pharmacology and Biochemistry

7.1 Pharmacodynamics

The pharmacodynamics of tapinarof are unknown.

▶ [DrugBank](#)

7.2 FDA Pharmacological Classification

1 of 2	
FDA UNII	84HW7D0V04
Active Moiety	TAPINAROF
Pharmacological Classes	Established Pharmacologic Class [EPC] - Aryl Hydrocarbon Receptor Agonist
Pharmacological Classes	Mechanisms of Action [MoA] - Aryl Hydrocarbon Receptor Agonists

FDA Pharmacology Summary

Tapinarof is an Aryl Hydrocarbon Receptor Agonist. The mechanism of action of tapinarof is as an Aryl Hydrocarbon Receptor Agonist.

[▶ FDA Pharm Classes](#)

2 of 2

Non-Proprietary Name

TAPINAROF

Pharmacological Classes

Aryl Hydrocarbon Receptor Agonist [EPC]; Aryl Hydrocarbon Receptor Agonists [MoA]

[▶ National Drug Code \(NDC\) Directory](#)

7.3 ATC Code



D - Dermatologicals

D05 - Antipsoriatics

D05A - Antipsoriatics for topical use

D05AX - Other antipsoriatics for topical use

D05AX07 - Tapinarof

[▶ WHO Anatomical Therapeutic Chemical \(ATC\) Classification](#)

7.4 Absorption, Distribution and Excretion



Absorption

No accumulation was observed with repeat topical application. Plasma concentration of tapinarof was below the quantifiable limits (BQL) of the assay (lower limit of quantification was 50 pg/mL) in 68% of the pharmacokinetic samples. On Day 1, mean $\pm$ SD values of C_{max} and AUC_{0-last} were 0.90 $\pm$ 1.4 ng/mL and 4.1 $\pm$ 6.3 ng.h/mL, respectively, following a mean daily dose of 5.23 g applied to a mean body surface area involvement of 27.2% (range 21 to 46%) in 21 subjects with moderate to severe plaque psoriasis. On Day 29, the mean $\pm$ SD C_{max} and AUC_{0-last} were 0.12 $\pm$ 0.15 ng/mL and 0.61 $\pm$ 0.65 ng.h/mL, respectively.

[▶ DrugBank](#)

Volume of Distribution

The V_{ss} of tapinarof is estimated to be from 1270 to 1500 mL/kg.

▶ [DrugBank](#)

7.5 Metabolism / Metabolites



Tapinarof is metabolized in the liver by multiple pathways including oxidation, glucuronidation, and sulfation in vitro. CYP1A2 and CYP3A4 appears to be the major enzyme involved in the hepatic metabolism of tapinarof, while CYP2C9, CYP2C19, and CYP2D6 play a minor role.

▶ [DrugBank](#)

7.6 Biological Half-Life



Due to the insufficient data about the elimination phase, the terminal half-life of tapinarof cannot be determined.

▶ [DrugBank](#)

7.7 Mechanism of Action



Tapinarof is a therapeutic aryl hydrocarbon receptor-modulating agent (TAMA) that binds to and activates the aryl hydrocarbon receptor (AhR). AhR is a ligand-dependent transcription factor that regulates gene expression in a variety of cell types, including macrophages, T-cells, antigen-presenting cells, fibroblasts, and keratinocytes. Upon binding to its ligand, AhR heterodimerizes with AhR nuclear translocator (ARNT) to form a complex with a high affinity for DNA binding. The AhR-ligand/ARNT complex can then bind to the specific DNA recognition sites to transcribe AhR-responsive genes. Additionally, AhR also exerts its effect through other transcription factors such as the nuclear factor κ B and nuclear factor erythroid 2-related factor 2 (Nrf2), a downstream product of AhR-induced transcription that has antioxidant properties. Dysregulation of AhR is one of the hallmarks of psoriasis, as psoriasis patients have a higher serum concentration of AhR compared to healthy individuals. Treatment of AhR ligands in vitro also results in a gene expression profile that is implicated in the pathogenesis of psoriasis. For instance, AhR activation causes the expansion and differentiation of Th17 and Th22, two major T cells responsible for releasing inflammatory cytokines IL-17 and IL-22. Additionally, AhR activation also recruits persistent skin resident memory T cells, thus contributing to the chronicity of psoriasis. However, the specific binding of tapinarof to AhR modulates a unique set of genes that are dysregulated in psoriasis, distinctive from other AhR ligands. Further, tapinarof also induces barrier protein expression, such as filaggrin, hornerin, and involucrin, to restore the skin barrier and epidermal function and decrease oxidative stress. It is currently unknown why AhR ligands like tapinarof can

reduce psoriatic inflammations in one setting but upregulate inflammatory genes in another setting. It is possible that the anti-inflammatory effect of tapinarof as an AhR agonist might be due to Nrf2. Although Nrf2 is a known downstream effector of AhR, not all AhR agonists activate this pathway. For instance, [2,3,7,8-tetrachlorodibenzo-p-dioxin](#), an AhR agonist, does not show any antioxidant activity after AhR activation. Therefore, it is hypothesized that the dual AhR/Nrf2 action of tapinarof is essential to the effect of tapinarof in treating psoriasis.

► [DrugBank](#)

8 Use and Manufacturing



8.1 Uses



8.1.1 Use Classification



Human Drugs -> FDA Approved Drug Products with Therapeutic Equivalence Evaluations (Orange Book) -> Active Ingredients

► [FDA Orange Book](#)

9 Safety and Hazards



9.1 Hazards Identification



9.1.1 GHS Classification



Pictogram(s)	 Environmental Hazard
Signal	<u>Warning</u>
GHS Hazard Statements	H400 (50%): Very toxic to aquatic life [<u>Warning</u> Hazardous to the aquatic environment, acute hazard] H410 (75%): Very toxic to aquatic life with long lasting effects [<u>Warning</u> Hazardous to the aquatic environment, long-term hazard] H413 (25%): May cause long lasting harmful effects to aquatic life [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

P273, P391, and P501

(The corresponding statement to each P-code can be found at the [GHS Classification](#) page.)

ECHA C&L Notifications Summary

Aggregated GHS information provided per 4 reports by companies from 3 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.

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.

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

9.1.2 Hazard Classes and Categories



Aquatic Acute 1 (50%)

Aquatic Chronic 1 (75%)

Aquatic Chronic 4 (25%)

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

10 Toxicity



10.1 Toxicological Information



10.1.1 Effects During Pregnancy and Lactation



● Summary of Use during Lactation

Tapinarof has not been studied during breastfeeding. Because it is poorly absorbed after topical application, it is considered a low risk to the nursing infant. Do not apply tapinarof directly to the nipple and areola and ensure that the infant's skin does not come into direct contact with the areas of skin that have been treated.

● Effects in Breastfed Infants

Relevant published information was not found as of the revision date.

● Effects on Lactation and Breastmilk

Relevant published information was not found as of the revision date.

► [Drugs and Lactation Database \(LactMed\)](#)

10.1.2 Protein Binding



Human plasma protein binding of tapinarof is approximately 99% in vitro.

► [DrugBank](#)

11 Associated Disorders and Diseases



► [Comparative Toxicogenomics Database \(CTD\)](#); [Open Targets](#); [Therapeutic Target Database \(TTD\)](#)

12 Literature



12.1 Consolidated References



▶ PubChem

12.2 NLM Curated PubMed Citations



▶ PubChem

12.3 Springer Nature References



► Springer Nature

12.4 Chemical Co-Occurrences in Literature



► PubChem

12.5 Chemical-Gene Co-Occurrences in Literature



[▶ PubChem](#)

12.6 Chemical-Disease Co-Occurrences in Literature

[▶ PubChem](#)

13 Patents



US10426743
US10195160
US10647649
US11458108
US11597692
US11590088
US11612573
US11617724
US11622945

[▶ DrugBank](#)

13.1 Depositor-Supplied Patent Identifiers



► PubChem

[Link to all deposited patent identifiers](#)

► PubChem

13.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

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

► PATENTSCOPE (WIPO)

13.3 FDA Orange Book Patents



► [FDA Orange Book](#)

13.4 Chemical Co-Occurrences in Patents



► [PubChem](#)

13.5 Chemical-Disease Co-Occurrences in Patents



► [PubChem](#)

13.6 Chemical-Gene Co-Occurrences in Patents



► PubChem

14 Interactions and Pathways



14.1 Chemical-Target Interactions



► ChEMBL; Comparative Toxicogenomics Database (CTD); Drug Gene Interaction database (DGIdb);...



▶ DrugBank

15 Biological Test Results



15.1 BioAssay Results



▶ PubChem

16 Taxonomy



The LOTUS Initiative for Open Natural Products Research: frozen dataset union wikidata (with metadata) | DOI:10.5281/zenodo.5794106

► LOTUS - the natural products occurrence database; Natural Product Activity and Species Source (...)

17 Classification



17.1 MeSH Tree



► Medical Subject Headings (MeSH)

17.2 NCI Thesaurus Tree





▶ NCI Thesaurus (NCIt)

17.3 ChEBI Ontology



▶ ChEBI

17.4 KEGG: Drug



▶ KEGG

17.5 KEGG: USP



▶ KEGG

17.6 KEGG: ATC



▶ KEGG

17.7 KEGG: Target-based Classification of Drugs



▶ KEGG

17.8 WHO ATC Classification System



► WHO Anatomical Therapeutic Chemical (ATC) Classification

17.9 ChemIDplus



► ChemIDplus

17.10 IUPHAR / BPS Guide to PHARMACOLOGY Target Classification



► IUPHAR/BPS Guide to PHARMACOLOGY

17.11 ChEMBL Target Tree



► ChEMBL

17.12 UN GHS Classification



► GHS Classification (UNECE)

17.13 NORMAN Suspect List Exchange Classification





▶ NORMAN Suspect List Exchange

17.14 EPA DSSTox Classification



▶ EPA DSSTox

17.15 The Natural Products Atlas Classification



▶ The Natural Products Atlas

17.16 LOTUS Tree



▶ LOTUS - the natural products occurrence database

17.17 FDA Drug Type and Pharmacologic Classification



► National Drug Code (NDC) Directory

18 Information Sources



FILTER BY SOURCE

ALL SOURCES



1. CAS Common Chemistry

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2-(1-Methylethyl)-5-[(1E)-2-phenylethenyl]-1,3-benzenediol

https://commonchemistry.cas.org/detail?cas_rn=79338-84-4

2. ChemIDplus

LICENSE

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

Tapinarof [USAN]

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0079338844>

ChemIDplus Chemical Information Classification

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

3. DrugBank

LICENSE

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https://www.drugbank.ca/legal/terms_of_use

Tapinarof

<https://www.drugbank.ca/drugs/DB06083>

4. EPA DSSTox

LICENSE

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

3,5-Dihydroxy-4-isopropyl-trans-stilbene

<https://comptox.epa.gov/dashboard/DTXSID301045262>

CompTox Chemicals Dashboard Chemical Lists

<https://comptox.epa.gov/dashboard/chemical-lists/>

5. European Chemicals Agency (ECHA)

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(E)-2-isopropyl-5-styrylbenzene-1,3-diol

<https://echa.europa.eu/substance-information/-/substanceinfo/100.274.186>

(E)-2-isopropyl-5-styrylbenzene-1,3-diol (EC: 838-014-1)

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/282996>

6. FDA Global Substance Registration System (GSRS)

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

TAPINAROF

<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/84HW7D0V04>

7. ChEBI

Benvitimod

<https://www.ebi.ac.uk/chebi/searchId.do?chebiId=ChEBI:215747>

ChEBI Ontology

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

8. FDA Pharm Classes

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

TAPINAROF

<https://dailymed.nlm.nih.gov/dailymed/browse-drug-classes.cfm>

9. LOTUS - the natural products occurrence database

LICENSE

The code for LOTUS is released under the GNU General Public License v3.0.

<https://lotus.nprod.net/>

3,5-Dihydroxy-4-isopropylstilbene

<https://www.wikidata.org/wiki/Q7638671>

LOTUS Tree

<https://lotus.naturalproducts.net/>

10. Open Targets

LICENSE

Datasets generated by the Open Targets Platform are freely available for download.

<https://platform-docs.opentargets.org/licence>

TAPINAROF

<https://platform.opentargets.org/drug/CHEMBL259571>

11. ChEMBL

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Access to the web interface of ChEMBL is made under the EBI's Terms of Use

(<http://www.ebi.ac.uk/Information/termsofuse.html>). The ChEMBL data is made available on a Creative Commons Attribution-Share Alike 3.0 Unported License (<http://creativecommons.org/licenses/by-sa/3.0/>).

<http://www.ebi.ac.uk/Information/termsofuse.html>

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL259571/

ChEMBL Protein Target Tree

<https://www.ebi.ac.uk/chembl/g/#browse/targets>

12. Comparative Toxicogenomics Database (CTD)

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<http://ctdbase.org/about/legal.jsp>

tapinarof

<https://ctdbase.org/detail.go?type=chem&acc=C571829>

13. Drug Gene Interaction database (DGIdb)

LICENSE

The data used in DGIdb is all open access and where possible made available as raw data dumps in the downloads section.

<http://www.dgldb.org/downloads>

TAPINAROF

<https://www.dgldb.org/drugs/rxcui:2602286>

14. IUPHAR/BPS Guide to PHARMACOLOGY

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The Guide to PHARMACOLOGY database is licensed under the Open Data Commons Open Database License (ODbL)

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<https://www.guidetopharmacology.org/about.jsp#license>

tapinarof

<https://www.guidetopharmacology.org/GRAC/LigandDisplayForward?ligandId=9686>

Guide to Pharmacology Target Classification

<https://www.guidetopharmacology.org/targets.jsp>

15. Therapeutic Target Database (TTD)

Tapinarof

<https://idrblab.net/ttd/data/drug/details/D03DMB>

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<https://www.accessdata.fda.gov/scripts/cder/daf/>

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<https://www.fda.gov/drugs/drug-approvals-and-databases/national-drug-code-directory>

22. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J478.929F

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J936.093J

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<https://www.kegg.jp/kegg/legal.html>

<https://www.kegg.jp/entry/D11365>

Therapeutic category of drugs in Japan

http://www.genome.jp/kegg-bin/get_htext?br08301.keg

USP drug classification

http://www.genome.jp/kegg-bin/get_htext?br08302.keg

Anatomical Therapeutic Chemical (ATC) classification

http://www.genome.jp/kegg-bin/get_htext?br08303.keg

Target-based classification of drugs

http://www.genome.jp/kegg-bin/get_htext?br08310.keg

24. Natural Product Activity and Species Source (NPASS)

3,5-Dihydroxy-4-Isopropylstilbene

<https://bidd.group/NPASS/compound.php?compoundID=NPC224527>

25. Metabolomics Workbench

Benvitimod

<https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=99721>

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NCI Thesaurus

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<https://www.nlm.nih.gov/research/umls/rxnorm/docs/termsofservice.html>

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<https://rxnav.nlm.nih.gov/id/rxnorm/2602286>

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<https://pharos.nih.gov/ligands/CWFD8WKL4TMF>

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<https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=19051389-328802919>

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https://www.whooc.no/atc_ddd_index/?code=D05AX07

ATC Code

https://www.whooc.no/atc_ddd_index/

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

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<https://www.ncbi.nlm.nih.gov/mesh/67571829>

MeSH Tree

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

36. GHS Classification (UNECE)

GHS Classification Tree

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

37. The Natural Products Atlas

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