

EPA's DSSTox Chemical Structure Database: A curated chemistry resource supporting computational toxicology research (Gulke et al.)

## Supplemental Material:

All websites accessed on 3/6/2019.

**Example 1.** PubChem record with multiple CAS RN and names synonyms assigned to "2-Octene". The trans (E) form of 2-Octene structure is shown, but three forms are listed as synonyms (cis, trans, mixture of cis/trans). DSSTox assigns each of these three forms to different substance records, each with its own substance name, CAS RN and structure.

<https://pubchem.ncbi.nlm.nih.gov/compound/5364448>

**PubChem** | OPEN CHEMISTRY DATABASE

Search PubChem

Compound Summary for CID 5364448

# 2-Octene

STRUCTURE VENDORS LITERATURE

PubChem CID: 5364448

Chemical Names: Trans-2-Octene; 13389-42-9; 2-OCTENE; (E)-2-Octene; (E)-oct-2-ene; 2-Octene, (E)-

Molecular Formula: C<sub>8</sub>H<sub>16</sub>

Molecular Weight: 112.216 g/mol

InChI Key: ILPBINAXDRFYPL-HWKANZROSA-N

Substance Registry: FDA UNII

Safety Summary: Laboratory Chemical Safety Summary (LCSS)

(E)-2-Octene is an acyclic olefin.

### 3.4.1 Depositor-Supplied Synonyms

1. trans-2-Octene	11. 2-Octene, (2E)-
2. 13389-42-9	12. 111-67-1
3. 2-OCTENE	13. cis-Octene-2
4. (E)-2-Octene	14. 2-Octene(mixed cis, trans isomers)
5. (E)-oct-2-ene	15. MFCD00009532
6. 2-Octene, (E)-	16. 2-Octene, cis-
7. UNII-G13G1YR8YW	17. trans-Oct-2-ene
8. oct-2-ene	18. 2-Octene (mixed cis, trans isomers)
9. G13G1YR8YW	19. EINECS 203-894-2
10. OCTENE-2	20. EINECS 236-463-2

### 3.3.1 CAS

111-67-1	from ChemIDplus, European Chemicals Agency (ECHA)
13389-42-9	from ChemIDplus, EPA DSSTox, European Chemicals Agency (ECHA)
7642-04-8	from DTP/NCI

**Example 2.** PubChem and ChemID records with incorrect metal assigned to structure.

<https://www.ncbi.nlm.nih.gov/pccompound?term=104199-51-1~%5Bsynonym%5D>

PubChem Compound 104199-51-1-[synonym]

Search results

Items: 2

1.  **104199-51-1; Ferrate(2-),** [3-(hydroxy-kappa O)-4-[[2-(hydroxy-kappa O)-4-hydroxy-5-[[2-methyl-5-((methylsulfonyl)amino)-4-[[4-(phenylamino)-3-sulfophenyl]azo]phenyl]azo]-3-(phenylazo)phenyl]azo-kappa N1]-7-nitro-1-naphthalenesulfonato(4-)-, sodium hydrogen; Ferrate(2-), [3-(hydroxy-kappa O)-4-[2-[2-(hydroxy-kappa O)-4-hydroxy-5-[2-[2-methyl-5-((methylsulfonyl)amino)-4-[2-[4-(phenylamino)-3-sulfophenyl]diazenyl]phenyl]diazenyl]-3-(2-phenyldiazenyl)phenyl]azo-kappa N1]-7-nitro-1-naphthalenesulfonato(4-)-, sodium hydrogen (1:1:1)]  
 MW: 1073.797 g/mol MF: C<sub>42</sub>H<sub>32</sub>FeN<sub>11</sub>NaO<sub>13</sub>S<sub>3</sub>  
 IUPAC name: sodium;4-[[5-[[4-(4-anilino-3-sulfophenyl)diazenyl]-5-(meth...]  
 Create Date: 2015-09-17  
 CID: 91867692  
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#)

2.  **104199-51-1; Ferrate(2-),** [3-(hydroxy-kappaO)-4-((2-(hydroxy-kappaO)-4-hydroxy-5-((2-methyl-5-((methylsulfonyl)amino)-4-((4-(phenylamino)-3-sulfophenyl)azo)phenyl)azo)-3-(phenylazo)phenyl)azo-kappaN1)-7-nitro-1-naphthalenesulfonato(4-)-, sodium hydrogen; Ferrate(2-), (3-(hydroxy-kappaO)-4-(2-(2-(hydroxy-kappaO)-4-hydroxy-5-(2-(2-methyl-5-((methylsulfonyl)amino)-4-(2-(4-(phenylamino)-3-sulfophenyl)diazenyl)phenyl)diazenyl)-3-(2-phenyldiazenyl)phenyl)azo-kappaN1)-7-nitro-1-naphthalenesulfonato(4-)-, sodium hydrogen (1:1:1)]  
 MW: 1079.482 g/mol MF: C<sub>42</sub>H<sub>30</sub>CuN<sub>11</sub>NaO<sub>13</sub>S<sub>3</sub>  
 IUPAC name: copper;sodium;4-[[5-[[4-(4-anilino-3-sulfonatophenyl)diazen...]  
 Create Date: 2007-07-03  
 CID: 16131308  
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#)

<https://chem.nlm.nih.gov/chemidplus/rn/104199-51-1>

TOXNET > ChemIDplus > Substance

ChemIDplus A TOXNET DATABASE

Substance Name: Ferrate(2-), (3-(hydroxy-kappaO)-4-(2-(2-(hydroxy-kappaO)-4-hydroxy-5-(2-(2-methyl-5-((methylsulfonyl)amino)-4-(2-(4-(phenylamino)-3-sulfophenyl)diazenyl)phenyl)diazenyl)-3-(2-phenyldiazenyl)phenyl)azo-kappaN1)-7-nitro-1-naphthalenesulfonato(4-)-, sodium hydrogen (1:1:1)  
 RN: 104199-51-1  
 InChIKey: PTXDUWIFJGIUPT-GROFPTGNSA-K

Structure Descriptors


InChI  
 1S/C42H33N11O13S3[Cu].[Na]/c1-23-17-32(47-45-26-13-16-30(38(18-26)69(64,65)66)43-24-9-5-3-6-10-24)33(52-67(2,59)60)20-31(23)46-48-34-21-35(42(56)40(41(34)55)51-44-25-11-7-4-8-12-25)49-50-39-28-15-14-27(53(57)58)19-29(28)37(22-36(39)54)68(61,62)63;/h3-22,43,52,54-56H,1-2H3,(H,61,62,63)(H,64,65,66);/q;+2,+1/p-3/b47-45+,48-46+,50-49+,51-44+;;  
[Download](#)

InChIKey  
 PTXDUWIFJGIUPT-GROFPTGNSA-K  
[Search the web for this InChIKey](#)

Smiles  
 [Cu+2]S([O-])(=O)(=O)c1cc(N=Nc2c(cc(N=Nc3cc(N=Nc4c5c(cc(cc5)[N+])([O-])=O)c(cc4[O-])S([O-])(=O)=O)c(c(N=Nc4cccc4)c3O)[O-])c(C)c2)NS(C)(=O)=O)ccc1Nc1cccc1.[Na+]  
[Download](#)

**Example 3.** Sample public supplier website listing both the correct structure-name-CAS and a mismatched synonym-structure-CAS.

<http://www.synquestlabs.com/product/id/72359.html>




# SYNQUEST LABORATORIES

Bringing creativity and innovation to fluorine chemistry

Search Catalog:  All

<b>Chemical Services</b>	<b>Perfluoro(3-oxapent-4-ene)sulfonyl fluoride</b>
Research Chemicals Catalog	Product #: 6362-2-03
Custom Synthesis & Manufacturing	Purity: 97%
Bulk Chemicals	Synonym: 2-Fluorosulfonyltetrafluoroethyl trifluorovinyl ether
Service & Support	CAS Number: 29514-94-1
	MDL Number: MFCD24842690
	Molecular Formula: C <sub>4</sub> F <sub>9</sub> O <sub>3</sub> S
	Molecular Weight: 280.09

<http://www.synquestlabs.com/product/id/27815.html>



# SYNQUEST LABORATORIES

Bringing creativity and innovation to fluorine chemistry

Search Catalog:  All

<b>Chemical Services</b>	<b>Perfluoro(4-methyl-3,6-dioxaoct-7-ene)sulfonyl fluoride</b>
Research Chemicals Catalog	Product #: 6362-2-01
Custom Synthesis & Manufacturing	Purity: 97%
Bulk Chemicals	Synonym: Perfluoro-2-(2-fluorosulfonylethoxy)propyl vinyl ether;
Service & Support	Perfluoro(3-oxapent-4-ene)sulfonyl fluoride; 2-Fluorosulfonyltetrafluoroethyl trifluorovinyl ether
Customer Support	CAS Number: 16090-14-5
	MDL Number: MFCD00798138
	Molecular Formula: C <sub>7</sub> F <sub>14</sub> O <sub>4</sub> S
	Molecular Weight: 446.12

**Example 4.** Sample DSSTox substance record with ambiguous synonyms and how they are mapped within DSSTox, also showing instance of mapped deleted CAS RN.

Ambiguous Synonym matched <b>null</b>  
You are viewing the record associated with DTXSID9022445  
CASRN: 620-92-8

Q bisphenol f

Other Possible Records

CAS	Reason
DTXSID4022446	Ambiguous Synonym matched
DTXSID00894123	Ambiguous Synonym matched

Systematic Name: 4,4'-Methylenediphenol  
MolFormula: C13H12O2  
InChI Key: PXKLMJQFEQBVLD-UHFFFAOYSA-N  
Smiles: [OC1=CC=C\(CC2=CC=C\(O\)C=C2\)C=C2](#)  
PubChem ID: [12111](#)  
Chemspider ID: [11614](#)

Substance ID: DTXSID9022445  
CAS: 620-92-8  
Name: Bis(4-hydroxyphenyl)methane

Substance type: Single Compound  
QC Level: DSSTox\_High  
Data Source: STN(DSSTox)

QC Notes:

Compound ID: DTXCID202445  
Chemical Shown: Tested Chemical

Internal QC Notes:

Source of CAS-Compound: STN(DSSTox)  
Double Stereo: None  
Chiral Stereo: None  
Chemical Form: Organic  
Organic Form: Parent

Associated Lists (75)

Synonyms (33)

Other Cas (1)

CAS-RN	Relationship	Source	Comments
1429425-30-8	Deleted	STN(DSSTox)	

Substance ID: DTXSID00894123  
CAS: 1333-16-0  
Name: Methylenebisphenol  
Substance Type: Mixture of Stereoisomers  
QC Level: DSSTox\_High  
Data Source: STN(DSSTox)  
Ill-defined substance

QC Notes:

Ambiguous Synonym matched  
You are viewing the record associated with DTXSID4022446  
CASRN: 2467-02-9

Q bisphenol f

Other Possible Records

CAS	Reason
DTXSID9022445	Ambiguous Synonym matched
DTXSID00894123	Ambiguous Synonym matched

Substance ID: DTXSID4022446  
CAS: 2467-02-9  
Name: 2,2'-Bisphenol F  
Substance Type: Single Compound  
QC Level: DSSTox\_High  
Data Source: STN(DSSTox)

**Example 5:** Sample relationship mappings in DSSTox for mixtures mapped to a component.

<https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID8020339#related-substances>

The screenshot shows the EPA DSSTox dashboard for Clophen A 30 (DTXSID8020339). The interface includes a navigation menu on the left with options like DETAILS, RELATED SUBSTANCES, and SYNONYMS. The main content area displays the searched chemical and its relationship to a component. The component is highlighted with a red box and labeled 'Component'. The chemical structure of 3,3'-Dichloro-1,1'-biphenyl is shown, along with its DTXSID, CASRN, and TOXCAS values.

**United States Environmental Protection Agency** Home Advanced Search Batch Search Lists Predictions Downloads Copy Share Submit Comment

## Clophen A 30

55600-34-5 | DTXSID8020339  
Searched by DSSTox Substance Id.

2 chemicals

Download / Send Show info: DTXSID CASRN TOXCAS Filter by: Name or CASRN Hide

Sort by: Relationship

**Searched Chemical**

1 related chemical structure with this substance

Clophen A 30  
DTXSID: DTXSID8020339  
CASRN: 55600-34-5  
TOXCAS: 0

**Component**

3,3'-Dichloro-1,1'-biphenyl  
DTXSID: DTXSID70872817  
CASRN: 2050-87-1  
TOXCAS: 0

<https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID7057864#related-substances>

The screenshot shows the EPA DSSTox dashboard for Clomiphene citrate (1:x) (DTXSID7057864). The interface includes a navigation menu on the left with options like DETAILS, RELATED SUBSTANCES, and SYNONYMS. The main content area displays the searched chemical and its relationship to a component. The component is highlighted with a red box and labeled 'Component'. The chemical structure of Clomiphene citrate (1:1) is shown, along with its DTXSID, CASRN, and TOXCAS values.

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## Clomiphene citrate (1:x)

43054-45-1 | DTXSID7057864  
Searched by DSSTox Substance Id.

2 chemicals

Download / Send Show info: DTXSID CASRN TOXCAS Filter by: Name or CASRN Hide

Sort by: Relationship

**Searched Chemical**

1 related chemical structure with this substance

Clomiphene citrate (1:x)  
DTXSID: DTXSID7057864  
CASRN: 43054-45-1  
TOXCAS: 0

**Component**

Clomiphene citrate (1:1)  
DTXSID: DTXSID8020337  
CASRN: 50-41-9  
TOXCAS: 271/661

**Example 6:** Sample relationship mappings in DSSTox for polymer mapped to a monomer, also showing representative structures provided for the non-structurable record on 2 public websites.

<https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID5025071#related-substances>

United States Environmental Protection Agency

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## 1,2-Dihydro-2,2,4-trimethylquinoline, polymer

26780-96-1 | DTXSID5025071  
Searched by DSSTox Substance Id.

DETAILS

**RELATED SUBSTANCES**

SYNONYMS

LINKS

BIOACTIVITY

EXPOSURE

HAZARD

COMMENTS

PROPERTIES

LITERATURE

2 chemicals

Download / Send Show info: DTXSID CASRN TOXCAST

Sort by: Relationship Filter by: Name or CASRN Hide

Searched Chemical

1 related chemical structure with this substance

1,2-Dihydro-2,2,4-trimethylquinoline, po...  
DTXSID: DTXSID5025071  
CASRN: 26780-96-1  
TOXCAST: 3/113

Monomer

1,2-Dihydro-2,2,4-trimethylquinoline  
DTXSID: DTXSID0025070  
CASRN: 147-47-7  
TOXCAST: 0

<https://pubchem.ncbi.nlm.nih.gov/compound/8981#section=2D-Structure>

PubChem OPEN CHEMISTRY DATABASE

Compound Summary for CID 8981

## 2,2,4-Trimethyl-1,2-dihydroquinoline

STRUCTURE VENDORS LITERATURE PATENTS BIOACTIVITIES

PubChem CID: 8981

Chemical Names: 2,2,4-Trimethyl-1,2-dihydroquinoline; 147-47-7; 1,2-DIHYDROACETONANIL; Flectol H More...

3.3.1 CAS 147-47-7

26780-96-1

from CAMEO Chemicals, ChemIDplus, DTP/NCI, EPA Chemicals under the TSCA, EPA DSSTox, ...

from ChemIDplus, EPA Chemicals under the TSCA, European Chemicals Agency (ECHA)

<https://chem.nlm.nih.gov/chemidplus/rn/25703-79-1>

NIH U.S. National Library of Medicine TOXNET TOXICOLOGY DATA NETWORK

Help FAQs TOXNET Fact Sheet Training Manual & Schedule

TOXNET > ChemIDplus > Substance

Registry Number equals 25703-79-1

Start New Query Modify Query Search History

Switch to Summary View

**Substance Name: Poly(2-hydroxypropyl methacrylate)**  
RN: 25703-79-1

InChIKey: VHSMLMUCYSAUQU-UHFFFAOYSA-N

Classification Code TSCA Flag XU (Exempt from Reporting under Chemical Data Reporting Rule)

Molecular Formula (C7-H12-O3)x-

Molecular Weight 144.1688

**Example 7.** Two sample DTXSID structures with advanced relative stereochemistry supported by v3000 mol files that are mapped by PubChem to v2000 structures in which the relative stereochemistry information is lost.

<https://comptox.epa.gov/dashboard/DTXSID6020561>

The screenshot shows the EPA dashboard for Endrin (DTXSID6020561). The main title is "Endrin" with the identifier "72-20-8 | DTXSID6020561" and "Searched by DSSTox Substance Id." The central image is a 3D ball-and-stick model of Endrin, a bicyclic organochlorine insecticide, with several chlorine atoms (Cl) and an oxygen atom (O) highlighted in green and blue. The stereochemistry is indicated with wedges and dashes, and some atoms are labeled "or1". To the left is a navigation menu with categories like "DETAILS", "EXECUTIVE SUMMARY", "PROPERTIES", "ENV. FATE/TRANSPORT", "HAZARD", "ADME", "EXPOSURE", "BIOACTIVITY", "SIMILAR COMPOUNDS", "GENRA (BETA)", "RELATED SUBSTANCES", "SYNONYMS", and "LITERATURE". To the right, there is a "Wikipedia" section with a brief description of Endrin as an organochlorine with the chemical formula  $C_{12}H_6Cl_6O$ , and an "Intrinsic Properties" section listing the molecular formula, average mass (380.9 g/mol), and monoisotopic mass.

<https://pubchem.ncbi.nlm.nih.gov/compound/12358480#section=2D-Structure>

The screenshot shows the PubChem compound summary for Hexadrin (CID 12358480). The main title is "Hexadrin" with the identifier "72-20-8" and "from CAMEO Chemicals, ChemIDplus, EPA DSSTox". The central image is a 2D chemical structure of Hexadrin, a bicyclic organochlorine insecticide, with several chlorine atoms (Cl) and an oxygen atom (O) highlighted in green and blue. The stereochemistry is indicated with wedges and dashes, and some atoms are labeled "or1". To the left is a navigation menu with categories like "STRUCTURE", "VENDORS", "PHARMACOLOGY", "LITERATURE", and "BIOACTIVITIES". Below the structure, there is a table of properties: PubChem CID: 12358480, Chemical Names: ENDRIN; Endricol; Endrex; Mendrin; Nendrin; Oktanex, Molecular Formula:  $C_{12}H_6Cl_6O$ , Molecular Weight: 380.895 g/mol, and InChI Key: DFBKLNHFCTMDC-GKRDHZSOSA-N. To the right, there is a section titled "3.4.2 Depositor-Supplied Synonyms" with a list of synonyms: 61. Endrin 1.6 EC, 62. Cmpd. 269, 63. 4-17-00-00525 (Beilstein Handbook Reference), 64. Endrin microg/mL in Cyclohexane, 65. CHEMBL2356732, and 66. DTXSID6020561. The last two items are highlighted with red boxes.

<https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID4023466>

**EPA** United States Environmental Protection Agency

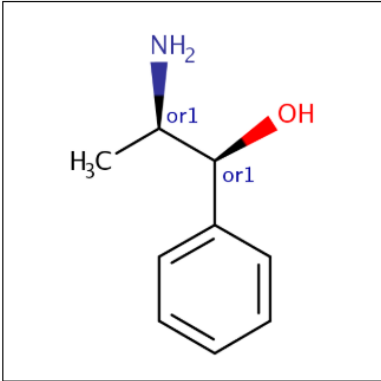
Home Advanced Search Batch Search Lists Predictions Downloads Copy Share Submit Comment Search

## Phenylpropanolamine

14838-15-4 | DTXSID4023466  
Searched by DSSTox Substance Id.

**DETAILS**

- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS



**Wikipedia**

Phenylpropanolamine (PPA) is a sympathomimetic agent which is used as a decongestant and appetite suppressant. It is commonly used in prescription and over-the-counter cough and cold preparations. In veterinary medicine, it is used to control urinary incontinence in dogs.

PPA is also known as  $\beta$ -hydroxyamphetamine, and is a member of the phenethylamine and amphetamine chemical classes. It is closely related to the cathinones ( $\beta$ -ketoamphetamines

...  
[Read more](#)

**Intrinsic Properties**

- Molecular Formula:  $C_9H_{13}NO$
- Mol File [Find All Chemicals](#)
- Average Mass: 151.209 g/mol
- [Isotope Mass Distribution](#)
- Monoisotopic Mass: 151.099714 g/mol

<https://pubchem.ncbi.nlm.nih.gov/compound/26934#section=Depositor-Supplied-Synonyms>

**PubChem** OPEN CHEMISTRY DATABASE

Search PubChem

Compound Summary for CID 26934

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## Norephedrine

Cite this

STRUCTURE VENDORS DRUG INFO PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

**PubChem CID:** 26934

**Chemical Names:** Norephedrine; Phenylpropanolamine; Rhindecron; DI-Norephedrine; (+)-Norephedrine; Dextrin  
[More...](#)

**Molecular Formula:**  $C_9H_{13}NO$

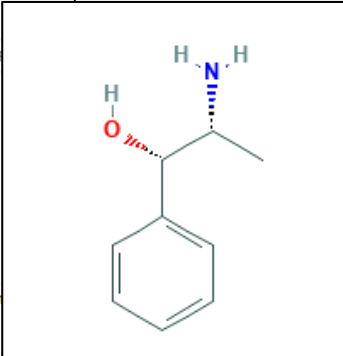
**Molecular Weight:** 151.209 g/mol

**InChI Key:** DLNKOYKMWOXYQA-VXNVDRBHSA-N

**Drug Information:** [Drug Indication](#) [Therapeutic Uses](#) [FDA UNII](#)

**Safety Summary:** [Laboratory Chemical Safety Summary \(LCSS\)](#)

Norephedrine is a sympathomimetic that acts mainly by causing release of NOREPINEPHRINE from some adrenergic receptors. It is most commonly used as a nasal vasoconstrictor and a



**3.3.1 CAS**

14838-15-4

from ChemIDplus, DTP/NCI, DrugBank, **EPA DSSTox**

**3.4.2 Depositor-Supplied Synonyms**

- 99. CHEMBL2092846
- 100. DTXSID4023466**