



SCIFINDERⁿ

A CAS SOLUTION

Quick Reference Guide

- 1 Login and Support
- 2-3 Interface and Reference search
- 4-5 Substance search and structure editor
- 6-7 Reaction search
- 8-9 Retrosynthesis Planner
- 10 Markush search and PatentPak
- 11 Suppliers search and ChemDoodle[®]

Login and Support

Login Details

- Login at <https://scifinder-n.cas.org>
- Use your existing SciFinder username and password
- Create a new SciFinderⁿ account for a new user: use the intranet SciFinder Registration URL of your institution

Learn More

- <https://www.cas.org/support/training/scifinder-n>

Training

- Contact aling@acs-i.org to organize your on-site or online session

Contact Customer Support

- Email help@cas.org to connect with a CAS Customer Center representative

Interface and Reference Search

Click on the logo to go to the home page

Access saved searches, Alerts and Combine.
Migrate SF-web assets

Access prior searches

Open What's New, MyCASProfile (i.e. Settings) and Online Help

Search Interface

SciFinderⁿ features a streamlined search interface.

Search

Enter the query

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use [Advanced Search](#) for Author, Journal, or Organization

Company or author name searches;
Access advanced substance search options

Launch the structure editor

Execute the search or press ENTER

Reference Search

The References display features visualizations, dynamic facets and an easy-to-use layout

- References are ranked and sorted by relevance by default
- You may save your searches, send a link or set-up alerts
- Filters allow you to focus the answers
- PatentPak shows the location of the indexed substances in the patent full-text

Load additional results for comprehensiveness

View indexed substances

View indexed reactions

View forward citations

Sort answers

Change how answers are displayed

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)
Load More Results

Filter by

- Document Type
 - Journal (138)
 - Patent (143)
 - Review (18)
 - Conference (1)
 - Dissertation (1)
- Substance Role
 - Adverse Effect (1)
 - Analytical Study (1)
 - Biological Study (102)
 - Preparation (33)
 - Process (1)

View All

Select filters to refine answers

References (282)

Sort: Relevance View: Partial Abstract

Substances Reactions Cited By

Download answers to file

Save results and set up alerts

Share answers by link

Click title to open reference detail

Access full-text options

View patent full text with chemistry annotation and location

Retrieve substance, reaction or citation data for this reference

3-Triazolylphenyl-substituted sulfide derivatives as acaricides and insecticides and their preparation

By: Alig, Bernd; Antons, Steffen; Voerste, Arnd; Goergens, Ulrich
World Intellectual Property Organization, WO2011020567 A1 2011-02-24 | Language: German, Database: CPlus

The invention relates to 3-triazolylphenyl-substituted sulfide derivatives of formula I, to their use as acaricides and insecticides for the control of animal pests and to methods for producing the same. Compounds of formula I wherein X is N and CA⁰ is H, halo, CN, alkyl, alkoxy, etc.; A¹ is CF₃ when X is N; A¹ is H, alkyl, haloalkyl, alkoxyalkyl, etc., when X is CA⁰; A² is H; B⁰ is H, amino, halo, CN, NO₂, etc.; B¹, B², and B³ are independently H, halo, CN, NO₂, alkyl, etc.; n is 0, 1 and 2; R¹ is H and alkyl; R² is CH₃, CF₃, CFCF₃, CH₂Cl etc. are claimed. Example compound II was pre...

View More

PATENTPAK Full Text Substances (653) Reactions (75) Cited By (5) Citation Map

Reference Detail and Search Operators

Publication source information

Patent

Patent Information

Patent Number
US20140005234

Publication Date
2014-01-02

Application Number
US2013-13919035

Application Date
2013-06-17

Kind Code
A1

Assignee
Unknown

Source
United States

Database Information
AN: 2014:3851
CAN: 160-144592
CAplus

Insecticidal N-substituted sulfilimine and **sulfoximine** pyridine N-oxides

By: Bland, Douglas C.; Ross, Ronald, Jr.; Johnson, Peter L.; Johnson, Timothy C.

Abstract: N-substituted sulfilimine and **sulfoximine** pyridine N-oxides were prepared according to the invention and their use in controlling insects and other invertebrates are provided. Further embodiments, forms, objects, features, advantages, aspects, and benefits shall become apparent from the description.

Access full-text options

PATENTPAK Viewer Full Text

Display of representative graphic

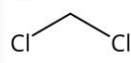
PDF displays original patent PDF
PDF+ displays full-text with table of indexed substances
Viewer displays interactive version of annotated full-text

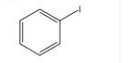
Patent Family

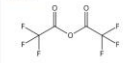
Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
US20140005234	English	A1	PDF PDF+ Viewer	2014-01-02	US2013-13919035	2013-06-17
CA2876184	English					2012-06-30
WO2014004086	English					2013-06-12
	English					2013-06-12
						2013-06-12

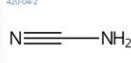
Substances

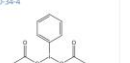
Substances (31)

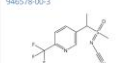
75-09-2
ClCCl
Dichloromethane
Pictorial: 
Role: Reactant, Reactant or Reagent

591-50-4
c1ccccc1I
Iodobenzene
Pictorial: 
Role: Reagent, Reactant or Reagent

407-25-0
FC(F)(F)C(=O)OC(F)(F)F
Trifluoroacetic anhydride
Pictorial: 
Role: Reactant, Reactant or Reagent

420-04-2
N#CN
Cyanamide
Pictorial: 
Role: Reagent, Reactant or Reagent

3240-34-4
CC1=CC=C(C=C1)OC(=O)C
Iodobenzene diacetate
Pictorial: 
Role: Reactant, Reactant or Reagent

946578-00-3
CS(=O)(=O)N
Sulfonamide
Pictorial: 
Role: Reactant, Reactant or Reagent

Subject matter and substance indexing is added by CAS scientists

- Concepts
- Substances
- Citations

View reference list of this document

Boolean Operators

Logical operators are available to define precise text queries

Use parentheses to group logical expressions such as OR'ed synonyms, e.g.:
(fungicide OR pesticide) AND strobilurin

AND Requires both words, phrases, or concepts to be present within the document



OR Requires either one or both words, phrases, or concepts to be present
Connect synonyms with OR



NOT Excludes documents from an answer set. Be careful when using the NOT operator, you cannot always assess the context of document texts



Wildcards, Masking

Wildcards and masking allow for more comprehensive retrieval and more precision respectively | Use in reference and substance name searches

Internal and right-hand truncation is available

***** Replaces 0 to any number of characters E.g.: polymorph* | immunoglobulin*conjugate*

? Replaces 0 or 1 character E.g.: 1,?-hexanediol

Terms masked with double quotes will be searched as a phrase, e.g.: "Programmed cell death protein"

Substance Name and Structure Searching

Name searches

Search with one or more substance names, identifiers, and document ID

Vanillin
57-92-1
Vanillin stearate
"Vanillin stearate" Vanillin
Vanillin*
WO2019020773

Finds Vanillin record
Finds Vanillin record, uses CAS Registry number as identifier
Finds 3 records: Vanillin, Vanillin stearate and Stearate
Finds 2 records: Vanillin stearate and Vanillin
Finds all names that start with the term Vanillin
Finds all indexed substances for this patent

Structure searches

A substance search returns results in an intuitive layout. The display highlights most relevant hits, critical property information and high-resolution images

Search

Search by Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Use **Advanced Search** for Molecular Formula, Substance Property, or Experimental Spectra

Enter query. For example, enter a chemical name

Access advanced substance search options: molecular formulas, properties and spectra line values

Click to draw new structure

Click query structure to edit

Checkmark to perform Markush search

Select type of structure match

Structure Match

- As Drawn (102)
- Substructure (4.3M)**
- Similarity (519)

Analyze Structure Precision

Identify tautomers or specific bond configurations

Commercial Availability

- Available (1.5M)
- Not Available (2.7M)

Reaction Role

- Product (588K)
- Reactant (140K)
- Reagent (394)
- Catalyst (396)
- Solvent (46)

Reference Role

- Adverse Effect (4,438)
- Analytical Study (8,123)
- Biological Study (1.6M)
- Combinatorial Study (2,775)
- Formation (2,623)

View All

Change sort criterion

Change amount of details displayed

Substances (4,303,959)

Sort: Number of Suppliers View Partial

References Reactions Suppliers Save

1 **90357-06-5**

C18H14F4N2O4S
Bicalutamide

3,844 References 202 Reactions 125 Suppliers

2 **149104-88-1**

Click Registry Number to open details

C7H9BO4S
[4-(Methylsulfonyl)phenyl]boronic acid

3 **373384-18-0**

Expands the answer to full view for that specific result

C7H9BO4S
(3-Methylsulfonylphenyl)boronic acid

4 **80-08-0**

Click on structure to open flyout window

C12H12N2
Dapsone

14K References 3,151 Reactions 107 Suppliers

Retrieve data related to substance

Substance Detail
Reactions (3,151)
Synthesize (87)
Create Retrosynthesis Plan
References (14K)
Suppliers (107)

Open editor with this structure

Download .sdf, .mol, .cxf, .png

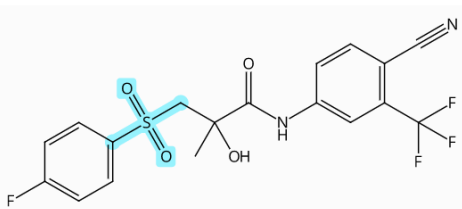
Reference Roles (also called substance roles) encode the new information reported about a substance

Substance Detail and Structure editor

Substance detail

Click on the image to show substance details with structure, molecular formula, properties and further data

CAS Registry Number
90357-06-5



Molecular formula in hill order
 $C_{18}H_{14}F_4N_2O_4S$

Systematic name
Propanamide, N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl-

Key Physical Properties	Value	Condition
Molecular Weight	430.37	-
Melting Point (Experimental)	190-195 °C (decomp)	-
Boiling Point (Predicted)	650.3±55.0 °C	Press: 760 Torr
Density (Predicted)	1.52±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.49±0.29	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Key properties

Other Names

Experimental Properties

Properties are either listed or available in linked source publications

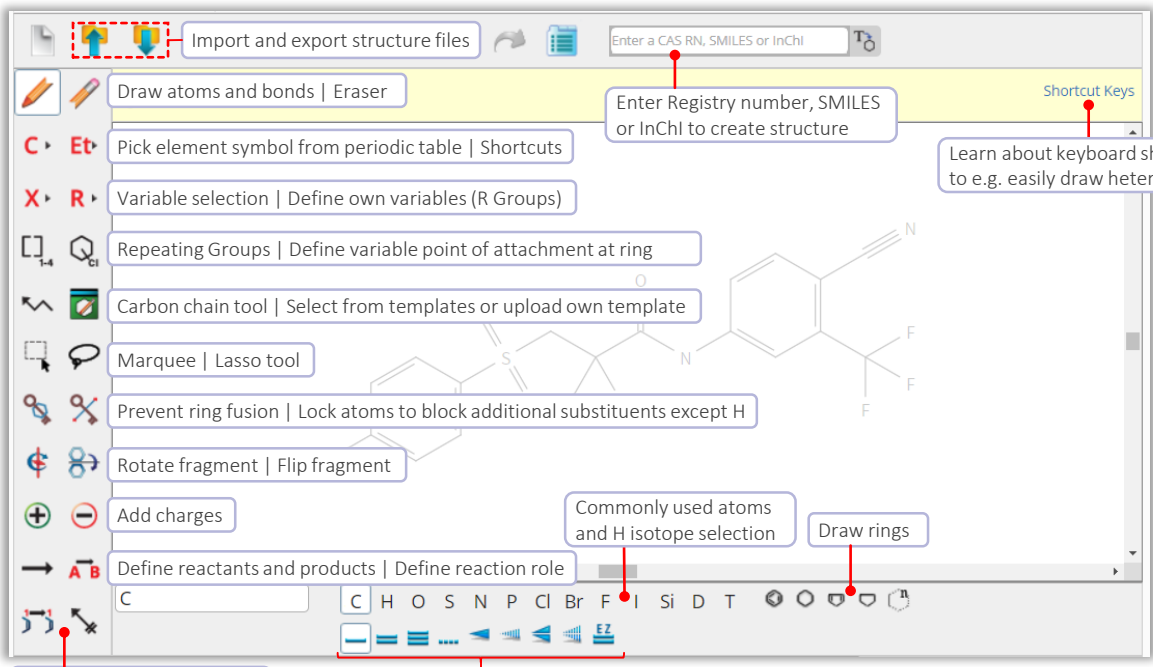
9 Other Names for this Substance

- (±)-4'-Cyano- α,α,α -trifluoro-3-[(p-fluorophenyl)sulfonyl]-2-methyl-m-lactotulidide
- Bicalutamide
- Casode
- Casodex
- Cosudex
- ICI 176334

Chemical names listed comprise systematic, trivial and trade names, as well as development codes. Names are extracted from analyzed publications.

CAS Draw editor

Define structure and reaction queries with the structure editor



Import and export structure files

Enter a CAS RN, SMILES or InChI

Shortcut Keys

Enter Registry number, SMILES or InChI to create structure

Learn about keyboard shortcuts to e.g. easily draw hetero atoms

Draw atoms and bonds | Eraser

Pick element symbol from periodic table | Shortcuts

Variable selection | Define own variables (R Groups)

Repeating Groups | Define variable point of attachment at ring

Carbon chain tool | Select from templates or upload own template

Marquee | Lasso tool

Prevent ring fusion | Lock atoms to block additional substituents except H

Rotate fragment | Flip fragment

Add charges

Commonly used atoms and H isotope selection

Draw rings

Define reactants and products | Define reaction role

Map atoms | Define bonds to be broken or formed

Draw bonds. Dotted line is unspecified bond

C H O S N P Cl Br F I Si D T

Reaction Searching

Reaction searches

Reactions queries can be substance names, CAS Registry Numbers, document identifiers, or chemical structures

- Reactions are grouped into schemes with identical reactants and products
- Reactions are sorted by yield within a scheme
- Find reactions by substance name, registry number, document identifier, chemical structure or reaction scheme

Search

All
Substances
Reactions
References
Suppliers

Select reactions

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

Enter a query...

Edit

Click on reaction query to edit

Edit Drawing Remove

Create Retrosynthesis Plan

Set Plan Options

Recent Search History

Reactions (6,410) View Expanded

References

Structure Match

As Drawn (61)
Substructure (6,410)
Similarity (27K)

View by structure match

Filter by

Yield
Number of Steps
Non-Participating Functional Groups
Experimental Protocols
Reaction Type
Stereochemistry
Reagent
Catalyst
Solvent
Commercial Availability
Reaction Notes
Stereoselective (1,191)
Regioselective (380)
Prophetic Reaction (267)
Chemoselective (209)
Biotransformation (87)
View All

Search Within Results

Source Reference
Document Type

Filter reaction results

Scheme 1 (30 Reactions) View substance information Steps: 1 Yield: 81-98%

View substance information

Yield range for displayed reactions

View suppliers Suppliers (93) Suppliers (131)

View substance information

Reaction Summary Steps: 1 Yield: 98%
1.1 Reagents: Hydrogen peroxide
Catalysts: Triaquea[μ-[1,3,5-benzenetricarboxylato(3-)-κO¹:κO¹]](μ₂-[1,3,5-benzenetricarbox...
Solvents: Ethanol, Acetonitrile; 1 h, rt → 100 °C
View Reaction Detail Experimental Protocols Full Text

Catalytic activity of HKUST-1 in the oxidation of trans-ferulic acid to vanillin
By: Yepez, Rebeca; et al
New Journal of Chemistry (2015), 39(7), 5112-5115

View reaction detail Steps: 1 Yield: 88%
1.1 Solvents: Water; 24 h, 40 °C
1.2 pH 5
View Reaction Detail PATENTPAK Full Text

Biotransformation of ferulic acid to vanillin by *Bacillus D LF-15161*
et al
China, CNT06957879 A 2017-07-18

View reaction detail Steps: 1 Yield: 81%
1.1 Solvents: Water; 24 h, 37 °C
View Reaction Detail PATENTPAK Full Text

Process for producing vanillin from immobilized microorganisms by surface culture
By: Asaff Torres, Ali; et al
World Intellectual Property Organization, WO2008130210 A1 2008-10-30

View All Reaction Summaries
Collapse Scheme

Reaction Details

Detailed information includes solvents, catalysts, reagents, conditions and experimental protocols extracted from the publication and its supplemental information.

SciFinderⁿ A CAS SOLUTION

Reactions

Reaction Detail

 (Scheme 10, Reaction 1 of 1) ← Prev Next →

Steps: 1
Yield: 42%

Double bond geometry shown

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Iodobenzene diacetate	Fe-TAML (complexes with lithium)	Acetone Diphenyl ether Water	1 h, 25 °C
2	Sodium sulfite	-	Water	-

CAS Reaction Number: 31-486-CAS-7572332

Notes

green chemistry-solvent, alternative preparation shown, other products also formed with 14% yield, selective oxidation

Experimental Protocols

MethodsNow™

Products

- Veratric acid, Yield: 7%
- 3,4-Dimethoxybenzaldehyde, Yield: 42%
- Diphenyl ether
- Water

Procedure

- Charge a dry, inert Radleys tube with the substrate (1 mmol), diphenyl ether (0.1-0.25 equivalent), Fe(TAm) Li (1 mol-%), and anhydrous acetone (5 ml), under argon atmosphere.
- Add the solution on a Radleys carousel and thermostated at 25 °C.
- Add iodobenzene diacetate (2 mmol) to the mixture.
- Stir the tube for 1 hour.
- Add saturated aqueous sodium sulfite (5 ml) to the mixture.
- Extract the mixture with ethyl acetate (3×5 ml).
- Dry the obtained solution on 3Å molecular sieves.

Transformation Ozonolysis

Scale milligram

Characterization Data

3,4-Dimethoxybenzaldehyde

State colorless oil.

Reaction reference

Reference

Fe(TAML)Li/(diacetoxyiodo) benzene-Mediated Oxidation of Alcohols: Evidence for Mild and Selective C-O and C-C Oxidative Cleavage in Lignin Model Transformations

By: Napoly, Francois; et al

European Journal of Organic Chemistry (2014), 2014(4), 781-787

Company/Organization

UMR CNRS 5246, Institut de Chimie et Biochimie Moléculaire et Supramoléculaire
Université Claude Bernard Lyon 1
Villeurbanne 69622
France

Retrosynthesis Planner

Launch plan generation

There are three options to launch SciFinderⁿ's retrosynthesis planner

- 1 Draw reaction structure and create plan from Edit icon
- 2 Open structure flyout window and start plan generation
- 3 Structured based reaction query without any results (not pictured)

Make sure *Reactions* is selected to view the **Create Retrosynthesis Plan** icon

Access plan options before launching the retrosynthesis tool

1 Draw reaction structure and create plan from Edit icon

2 Open structure flyout window and start plan generation

Open plan

The Experimental Plan is available within a few seconds. As soon as the calculation of the Predictive Retrosynthesis Plan is finished, a notification will pop up in that retrosynthetic plan. You will also be informed via email.

Access plan options from the top bar

Red lines mark experimental steps, i.e. those reported in the literature

Review alternative disconnections

Switch predicted steps on/off

Green dotted lines indicate predicted steps

Powered by ChemPlanner[®]

Estimated Yield: 28%
Overall Price: \$1,217.28
(USD per 100 grams)

Commercially Available: B, D, E, F, G, H, I, J

Alternative Steps and Plan Options

Alternative steps

Provide an overview of all experimental and predicted disconnections
Evidence reactions are displayed as a reaction answer set
Access Evidence Reactions from the **1** link in the steps overview or **2** the alternative reaction scheme

The screenshot displays the 'Alternative Steps' section of the ChemPlanner interface. On the left, a list of alternative steps is shown, with step **A → B + C** selected. A callout box labeled **1** points to the 'Evidence (2,059)' link for this step. The main area shows a list of 48 alternative steps, with step **7 of 48** selected. A callout box labeled **2** points to the 'Evidence (88)' link for this step. A detailed view of the selected step shows a reaction scheme with a yield of 90%. A callout box labeled 'Evidence reactions for predicted disconnection' points to the reaction details, which include reagents, solvents, and temperatures. A callout box labeled 'Select alternative - the plan will be reorganized' points to the 'Select' button in the reaction details.

Plan options

Edit plan options to...

- Change the synthetic depth
- Maintains connectivity of bonds through the entire synthetic route
- Define bonds to be broken in the first disconnection
- Create a plan with potentially more alternatives, e.g. for poly- or heterocyclic molecules

The screenshot displays the 'Plan Options' section of the ChemPlanner interface. The 'Select Synthetic Depth' section has a callout box labeled 'Change number of disconnections in the plan' pointing to the depth selection radio buttons (1, 2, 3, 4). The 'Break and Protect Bonds' section has a callout box labeled 'Maintains connectivity of bonds through the entire synthetic route' pointing to the 'Break Bond' and 'Protect Bond' buttons. A callout box labeled 'Break bond in first disconnection' points to the 'Break Bond' button. A callout box labeled 'Select uncommon or rare rules supported by fewer literature examples' points to the 'Rare' radio button in the 'Set Rules Supporting Predicted Reactions' section. A callout box labeled 'Let us know if you have any questions or comments' points to the 'Feedback' button at the bottom right.

Markush Searching and PatentPak

Markush searching

Markush structure searches can be performed by using the Search Patent Markush option while in Substances search mode

The screenshot shows the SciFinder interface with search results for patent claims. On the left, there are filters for 'Patent Markush Match' (As Drawn (93), Substructure (115)) and 'Filter by Patent Office' (World Intellectual Property Organization (55), United States (25), European Patent Organization (8), United Kingdom (2), Canada (1)). The main area displays three patent claims with chemical structures and associated text. Callouts point to various features: 'Markush search type' points to the 'As Drawn' filter; 'Filter by patent authority' points to the 'Patent Office' filter; 'Markush search option' points to the 'Search Patent Markush' checkbox; 'Markush definition location' points to the 'Patent claim 12' header; 'Link to PatentPak viewer' points to the 'Full Text' dropdown; and 'Link to 3rd party full text options' points to the 'Full Text' dropdown for a specific claim.

PatentPak Viewer

The screenshot shows the PatentPak Viewer interface. At the top, there are controls for 'Display controls', 'Download PDF', and 'Download PDF including chemistry annotations'. The main area displays patent claims with chemical structures. Callouts point to various features: 'Display controls' points to the 'PAGE' and 'ZOOM' controls; 'Download PDF' points to the 'PDF' button; 'Download PDF including chemistry annotations' points to the 'PDF+' button; 'Link to location of substance in patent' points to the 'Page 12' link; 'Highlighted key substance is marked' points to the highlighted 'Li' in the patent text; 'Link to related information' points to the 'Substance Detail' menu; 'Marks key substance curated by CAS scientists' points to the 'Li' structure; and 'Key substances identified in the patent are annotated' points to the 'Analyst Markup Locations' section.

Suppliers Searching and ChemDoodle®

Suppliers searching

Suppliers searching allows for direct access to chemical catalog information based on chemical structure, names or other identifiers

The screenshot shows the SciFinder Suppliers search interface. The search term is "hydrogen peroxide*35%*". The results are sorted by Relevance. The first result is from TCI Research Chemicals (SGD) Singapore, with a link to detail. The second result is from Alfa Aesar, United States. A "Supplier Detail" window is open for TCI Research Chemicals (SGD), showing contact information, catalog details, and an order link. The chemical structure of hydrogen peroxide is shown as HO—OH.

Suppliers (9)

Supplier	Substance	Purity	Purchasing Details
1 TCI Research Chemicals (SGD) Singapore	7722-84-1 Hydrogen Peroxide (35% in Water)		Order From Supplier 300 mL, SGD 24.00
2 TCI Research Chemicals Japan			
3 Alfa Aesar Alfa Aesar United States			

Sort options

- Sort: Relevance
- Relevance
- Supplier: A to Z
- Supplier: Z to A
- Ships Within
- Purity

Preferred/non-preferred supplier tagging

Link to detail

Supplier Detail (1 of 9)

TCI Research Chemicals (SGD)

Web: <https://www.tcichemicals.com/en/sg/>

Email: AskUs@teehaichem.com.sg

Phone: +65-68625655

Contact information

Substance Information

CAS Registry Number: 7722-84-1

CAS Name: Hydrogen peroxide

Chemical Name: Hydrogen Peroxide (35% in Water)

Order Number: H1222

Quantity, Price: 300 mL, SGD 24.00

Bulk Available

Catalog details

Stock Status: Maintained in stock

Ships Within: 1 week

Pricing Information: 19 Mar 2020

Order From Supplier

Order link

Chemical Structure: HO—OH

ChemDoodle®

ChemDoodle structure editor is available in addition to the standard CASdraw editor. ChemDoodle is useful for tablets and mobile devices.

The screenshot shows the ChemDoodle structure editor interface. The editor is open over a search result for hydrogen peroxide. The interface includes a toolbar with various drawing tools, a menu with options like "Center", "Flip fragment", "Cut | Copy | Paste", "Clear | Eraser", "Labeling", "Draw bonds", "Draw rings", "Add charges", "Chain tool", "Repeating groups", "Variable point of attachment", "Lock atoms/chains/rings", "Make reaction", "Reaction mapping", and "Break/form bonds". The chemical structure of hydrogen peroxide is shown in the center of the editor.

Center

Flip fragment

Cut | Copy | Paste

ChemDoodle

Lasso

Model with CAS Registry Number

Clear | Eraser

Undo | Redo

Templates

Open | Save

Zoom

Labeling

Draw bonds

Draw rings

Add charges

Chain tool

Repeating groups

Variable point of attachment

Lock atoms/chains/rings

Make reaction

Reaction mapping

Break/form bonds

ChemDoodle®

OK

Cancel