



SciFinder-n

THE MOST COMPREHENSIVE
CHEMISTRY AND CHEMICAL
ENGINEERING DATABASE

SEARCH BY SUBSTANCES,
REACTIONS (ORGANIC),
REFERENCES, AND MORE

ABOUT

[HTTPS://WWW.CAS.ORG/SOLUTIONS
/CAS-SCIFINDER-DISCOVERY-
PLATFORM/CAS-SCIFINDER-N](https://www.cas.org/solutions/cas-scifinder-discovery-platform/cas-scifinder-n)



Searching for...

All

Substances

Reactions

References

Suppliers

Sequences

Retrosynthesis

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

DMSO

AND

Molecular Formula

+ Add Advanced Search Field

Examples: C₆H₆ | (C₈H₈)_x | C₂₂H₂₆CuN₂O₅.C₂H₃N[Learn more about SciFinder[®] Advanced Search.](#)

SciFinder-n – Searching for DMSO as a Substance

[Return to Home](#)

Substances search for "DMSO"

References ▾

Reactions ▾

Suppliers ▾

Filter Behavior

Filter by

Exclude

Reaction Role

Product (2)

Reactant (1)

Reagent (1)

Catalyst (1)

Solvent (1)

Reference Role

Uses (14)

Biological Study (13)

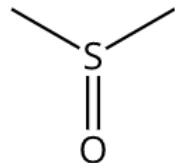
Therapeutic Use (10)

Pharmacological Activity (5)

Technical or Engineered

 15 Results 1

67-68-5

C₂H₆OS

DMSO

 125K
References 837K
Reactions 349
Suppliers 2

110070-80-9

Image Not Available

Notes: Described as an agent related to
DMSO (Pharmacia Inc.)

Unspecified

Sulphopentosan

 2
References 0
Reactions 0
Suppliers 4

1692892-06-0

 5

623574-38-9

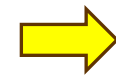
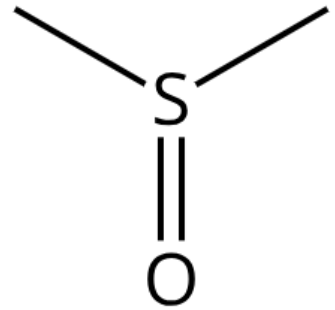
SciFinder-n –
Substance
search results
for DMSO

Return to Results

Prev (1 of 15) Next

CAS Registry Number: 67-68-5

References (127K) Reactions (848K) Suppliers (352) Download Email Save



- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Predicted Properties
- Predicted Spectra
- Regulatory Information
- GHS Hazard Statements
- Additional Details

C₂H₆OS
Methane, 1,1'-sulfinylbis- (ACI)



SciFinder-n Substance Details – Includes links to References, Reactions, and Suppliers, plus Other Names & Identifiers, Properties, Spectra, Regulatory Information.

Code, statements, and pictograms from the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) became available in SF-n on June 26, 2023.

GHS Hazard Statements



Code	Hazard Statement	Source
H432	Toxic to terrestrial vertebrates	Fisher Scientific (Lomb)
H373	May cause damage to organs; through prolonged or repeated exposure	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria, TCI America, Tokyo Chemical Industry Co (Tokyo Kasei Kogyo Co)
H371	May cause damage to organs	Expert Curated, Japan GHS Classifications (Japanese)
H351	Suspected of causing cancer	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria

Selected GHS Hazard Statements for DMSO

[Return to Home](#)

Reactions for 67-68-5

References



Save and Alert

Filter Behavior

Filter by

Exclude

Substance Role

- Product (868)
- Reactant (16K)
- Reagent (59K)
- Catalyst (3,117)
- Solvent (769K)

Yield

- 90-100% (79K)
- 80-89% (95K)
- 70-79% (89K)
- 50-69% (128K)
- 30-49% (71K)

[View All](#) 837,191 Results

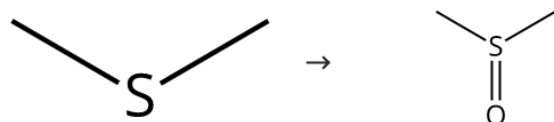
Group: By Scheme

Sort: Relevance

View: Expanded

Scheme 1 (275 Reactions)

Steps: 1 Yield: 100%

[Suppliers \(67\)](#)[Suppliers \(349\)](#) 31-614-CAS-34658989

Steps: 1 Yield: 100%

Titanium(IV) Alkoxide-Carbamate Complexes: Synthesis and Catalytic Potential in H₂O₂-Oxidation of Organic Sulfides

1.1 Reagents: [Hydrogen peroxide](#)
Solvents: [Methanol-d₄](#), [Water](#); 2 h, 25 °C

By: [Bresciani, Giulio](#); et al
European Journal of Inorganic Chemistry (2022), 2022(30), e202200402

[Full Text](#)

SciFinder-n – Viewing Reactions

Filter Behavior

Filter by

Exclude

^ Substance Role

- Product (868)
- Reactant (16K)
- Reagent (59K)
- Catalyst (3,117)
- Solvent (769K)

^ Yield

- 90-100% (79K)
- 80-89% (95K)
- 70-79% (89K)
- 50-69% (128K)
- 30-49% (71K)

[View All](#)

^ Number of Steps

- 1 (836K)
- 2 (135)
- 3 (92)
- 4 (16)
- 5 (2)

^ Non-Participating Functional Groups

- Halide (253K)
- Alkene (232K)
- Ether (225K)
- Cyclic alkene (176K)
- Amide (143K)

[View All](#)

^ Reaction Mapping

- Mapping Data Available (774K)
- No Mapping Data Available (62K)

^ Reaction Scale

- Milligram (134K)
- Gram (33K)
- Kilogram (93)
- No Scale Provided (668K)

^ Experimental Protocols

- Synthetic Methods (275K)
- Experimental Procedure (175K)

^ Reaction Type

^ Stereochemistry

^ Reagent

^ Catalyst

^ Solvent

^ Commercial Availability

^ Reaction Notes

- Regioselective (78K)
- Stereoselective (64K)
- Photochemical (31K)
- Chemoselective (27K)
- Green Chemistry (25K)

[View All](#)

^ Search Within Results

Source Reference

^ Document Type

^ Language

^ Publication Year

^ Organization

^ Publication Name

^ CA Section

SciFinder-n – Options for Filtering Reaction Search Results

Reaction Notes

By Count

Alphanumeric

- Regioselective (78K)
- Stereoselective (64K)
- Photochemical (31K)
- Chemoselective (27K)
- Green Chemistry (25K)
- Combinatorial (24K)
- Solid-Supported Reaction (23K)
- Microwave Irradiation (22K)
- Biotransformation (12K)
- Prophetic Reaction (12K)
- Enzymic (11K)
- Solid-Supported Catalyst (5,720)
- Thermal (5,569)
- In The Dark (5,016)
- Green Chemistry-Catalyst (4,022)
- Green Chemistry-Reagent (3,853)
- Solid-Supported Reagent (3,736)
- Electrochemical (2,968)
- Safety (2,741)
- Ultrasound (2,689)
- High Pressure (1,912)
- Green Chemistry-Process Simplification (1,271)
- Green Chemistry-Solvent (1,000)
- Low Pressure (605)
- Radiochemical (558)
- Green Chemistry-Waste Reduction (491)
- Anaerobic (441)
- Fermentation (314)
- Failed Reaction (198)
- Solid State (120)
- Explosion (110)
- Green Chemistry-Renewable Feedstock (92)
- Gas Phase (15)

Apply

Cancel

SciFinder-n –
Reaction Notes

🧪 Reactions for 67-68-5

References ▾



Save and Alert

Filter Behavior

Filter by

Exclude

Substance Role

- Reactant (27)
- Reagent (4)
- Catalyst (20)
- Solvent (408)

Yield

- 90-100% (97)
- 80-89% (58)
- 70-79% (68)
- 50-69% (96)
- 30-49% (51)

[View All](#)

Number of Steps

- 1 (444)

Filtering:

Experimental Protocols: Experimental Procedure ✕

[Clear All Filters](#)

Reaction Notes: 2 Selected ✕

Document Type: Journal ✕

 444 Results

Group: By Scheme ▾

Sort: Relevance ▾

View: Expanded ▾

Scheme 1 (1 Reaction)

Steps: 1 Yield: 100% ⋮



Suppliers (4)

[31-614-CAS-25648469](#)

Steps: 1 Yield: 100%

[Efficient Access to Orthoquinols and Their \[4 + 2\] Cyclodimers via SIBX-Mediated Hydroxylative Phenol Dearomatization](#)

1.1 Reagents: [Benzoic acid](#), [Isophthalic acid](#), [2-Iodoxybenzoic acid](#)
Solvents: [Dimethyl sulfoxide](#); 2 h, rt

By: Lebrasseur, Nathalie; et al
Journal of Organic Chemistry (2007), 72(16), 6280-6283

Full Text ▾

Experimental Protocols

SciFinder-n Search Results – 1st Reaction Scheme



Experimental Protocols

Synthetic Methods

Experimental Procedure

Products	2-Hydroxy-2-methyl-1(2H)-naphthalenone , Yield: 100%
Reactants	2-Methyl-1-[(trimethylsilyl)oxy]naphthalene
Reagents	Benzoic acid Isophthalic acid 2-Iodoxybenzoic acid
Solvents	Dimethyl sulfoxide
Procedure	<ol style="list-style-type: none">1. Treat the trimethylsilylated 2-methylnaphthol (0.2 mmol) in DMSO (1 mL) with SIBX (255 mg, 0.5 mmol, i.e., 2.5 equivalent of IBX) at room temperature for 2 hours.2. After 2 hours, dilute the reaction mixture with EtOAc (20 mL).3. Wash the reaction mixture with saturated aqueous NaHCO₃ (3 × 5 mL) and brine (5 mL).4. Dry the reaction mixture over Na₂SO₄.5. Filter the reaction mixture.6. Evaporate the reaction mixture.
Scale	milligram


Characterization Data

^ [2-Hydroxy-2-methyl-1\(2H\)-naphthalenone](#)

State red oil.

CAS Method Number 3-614-CAS-2488692

Reaction Notes

chemoselective, safety (stabilized IBX used 1st stage) 

SciFinder-n – Experimental Protocols > Synthetic Methods & Reaction Notes

Alternative Steps (0)

Experimental Protocols

Synthetic Methods

Experimental Procedure



JOC
The Journal of Organic Chemistry

Method B. Treatment of the trimethylsilylated 2-methylnaphthol **11b** (50 mg, 0.2 mmol) in DMSO (1 mL) with SIBX (255 mg, 0.5 mmol, i.e., 2.5 equiv of IBX) was run at room temperature for 2 h, after which time the reaction mixture was diluted with EtOAc (20 mL), washed with saturated aqueous NaHCO₃ (3 × 5 mL), and brine (5 mL), dried over Na₂SO₄, filtered and evaporated to furnish orthoquinol **12** (35 mg, 100%) as a red oil.

Reaction Notes

chemoselective, safety (stabilized IBX used 1st stage)

SciFinder-n – Experimental Protocols > Experimental Procedure

Searching for...

All

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Retrosynthesis

References

Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

10.1021/acs.analchem.7b00233



Draw



AND ▾

Author Name ▾

Enter last name, first name middle name.*Example: Schubert, J A*

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SciFinder-n – References Search using DOI (Digital Object Identifier) of Paper

CAS SciFinder[®] 10.1021/acs.analchem.7b00233

References search for "10.1021/acs.analchem.7b00233"

Substances Reactions Citing Knowledge Graph Save and Alert

Filter Behavior: Filter by Exclude

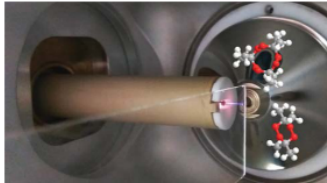
Document Type: Journal (1)

Language: English (1)

Publication Year: 2012 to 2022

1 Result View: Full Abstract

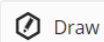
Determination of Peroxide Explosive TATP and Related Compounds by Dielectric Barrier Discharge Ionization-Mass Spectrometry (DBDI-MS)
 By: Hagenhoff, Sebastian; Franzke, Joachim; Hayen, Heiko
 Analytical Chemistry (Washington, DC, United States) (2017), 89(7), 4210-4215 | Language: English, Database: CPlus and MEDLINE | Analytical Methods



Dielec. barrier discharge ionization-mass spectrometry (DBDI-MS), which is based on the use of a low temperature helium plasma as ionization source, is used for the determination of trace amounts of triacetone triperoxide (TATP) and its homolog diacetone diperoxide (DADP) from surfaces. TATP is observed as $[M+NH_4]^+$ adduct, whereas DADP is observed as $[M+O+NH_4]^+$. Measurement of DADP with varying deuteration degrees (DADP, DADP- d_6 , and DADP- d_{12}) indicates that DADP undergoes oxidation when ionized by DBDI. If acetonitrile is used as deposition solvent, TATP tends to show fragmentation and is not only detected as $[M+NH_4]^+$ but as $[M-CH_4+NH_4]^+$ and $[M-C_2H_4+NH_4]^+$ as well. Quantification of TATP solutions from glass surfaces by DBDI-MS, using TATP-3,6,9- ^{13}C as internal standard, was done and validated using an LC/APCI-MS method. Achievable limits of detection (LOD) for TATP are equivalent to the deposition of 15 ng TATP and are comparable with other ambient desorption/ionization mass spectrometric techniques like desorption electrospray ionization (DESI).

Full Text Substances (2) Reactions (0) Citing (32) Citation Map

SciFinder-n Search Results for DOI

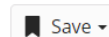


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Prev (1 of 1) Next

Determination of Peroxide Explosive TATP and Related Compounds by Dielectric Barrier Discharge Ionization-Mass Spectrometry (DBDI-MS)

Substances (2) Reactions (0) Citing (32) Citation Map



JOURNAL

Source

Analytical Chemistry (Washington, DC, United States)
Volume: 89
Issue: 7
Pages: 4210-4215
Journal; Article
2017
DOI:
[10.1021/acs.analchem.7b00233](https://doi.org/10.1021/acs.analchem.7b00233)

CODEN: ANCHAM
E-ISSN: 1520-6882
ISSN-L: 0003-2700

Database Information

AN: 2017:366343
CAN: 166:330172
PubMed ID: 28253619
CAplus and MEDLINE

Company/Organization

By: Hagenhoff, Sebastian; Franzke, Joachim ; Hayen, Heiko

Dielec. barrier discharge ionization-mass spectrometry (DBDI-MS), which is based on the use of a low temperature helium plasma as ionization source, is used for the determination of trace amounts of triacetone triperoxide (TATP) and its homolog diacetone diperoxide (DADP) from surfaces. TATP is observed as $[M+NH_4]^+$ adduct, whereas DADP is observed as $[M+O+NH_4]^+$. Measurement of DADP with varying deuteration degrees (DADP, DADP-d₆, and DADP-d₁₂) indicates that DADP undergoes oxidation when ionized by DBDI. If acetonitrile is used as deposition solvent, TATP tends to show fragmentation and is not only detected as $[M+NH_4]^+$ but as $[M-CH_4+NH_4]^+$ and $[M-C_2H_4+NH_4]^+$ as well. Quantification of TATP solutions from glass surfaces by DBDI-MS, using TATP-3,6,9-¹³C as internal standard, was done and validated using an LC/APCI-MS method. Achievable limits of detection (LOD) for TATP are equivalent to the deposition of 15 ng TATP and are comparable with other ambient desorption/ionization mass spectrometric techniques like desorption electrospray ionization (DESI).



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Format

Keywords: peroxide explosive compound dielec barrier discharge ionization mass spectrometry

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Direct Determination of Peroxide Explosives on Polycarbazole/Gold Nanoparticle-Modified Glassy Carbon Sensor Electrodes...

Analytical Chemistry (Washington, DC, United States) (2022), 94(50), 17662-17669 | Language: English, Database: CAPlus and MEDLINE

Electrochemical determination of triacetone triperoxide (TATP) using polycarbazole modified glassy carbon electrode

Abstracts of Papers, ACS Spring 2021 (2021), No pp. given | Language: English, Database: CAPlus

Determining the vapor pressures of diacetone diperoxide (DADP) and hexamethylene triperoxide diamine (HMTD)

Propellants, Explosives, Pyrotechnics (2009), 34(6), 539-543 | Language: English, Database: CAPlus

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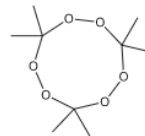
^ Concepts

Explosives

^ Substances

Substances (2)

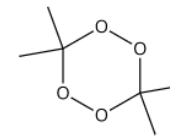
17088-37-8



$C_9H_{18}O_6$
Triacetone triperoxide

Role: Analyte, Technical or Engineered Material Use, Analytical Study, Uses

1073-91-2



$C_6H_{12}O_4$
Diacetone diperoxide

Role: Analyte, Technical or Engineered Material Use, Analytical Study, Uses

^ Analytical Methods

Title

CAS Method Number

Analysis of Triacetone triperoxide by Dielectric spectroscopy

[1-121-CAS-276727](#)

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Find substances by Name, CAS Registry Number, or chemical structure; find reactions; and then filter or refine results to reactions that have safety notes and/or experimental details.



Find substances, view references, and then refine by topics to further focus results.



Search by keyword in references to find names, functional groups, or compounds class names mentioned in abstracts or as index terms.



Search the DOI from a relevant article and see how it is indexed in SciFinder-n so that you are more easily able to find other, similar papers.



For SF-n users, start with the CAS Lexicon that includes both controlled subject terms as well as functional groups and classes of compounds.