



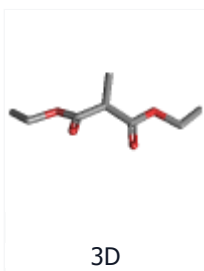
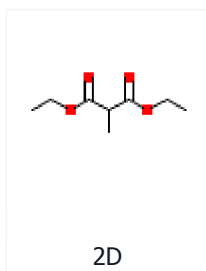
COMPOUND SUMMARY

Diethyl methylmalonate

PubChem CID

11857

Structure



Chemical Safety



Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula

C₈H₁₄O₄

Synonyms

DIETHYL METHYLMALONATE

609-08-5

Diethyl 2-methylmalonate

diethyl 2-methylpropanedioate

Methylmalonic acid diethyl ester

[View More...](#)

Molecular Weight

174.19 g/mol

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Dates

Create:2005-03-26

Modify:2024-09-20

Contents

Title and Summary	
1 Structures	▼
2 Names and Identifiers	▼
3 Chemical and Physical Properties	▼
4 Spectral Information	▼
5 Related Records	▼
6 Chemical Vendors	
7 Use and Manufacturing	▼
8 Safety and Hazards	▼
9 Literature	▼
10 Patents	▼
11 Biological Test Results	▼
12 Classification	▼
13 Information Sources	

1 Structures

?

↗

1.1 2D Structure

?

↗

🔍

🖼️

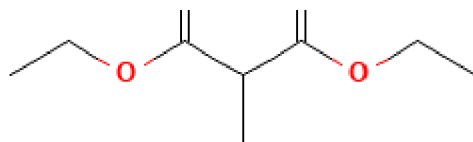
⬇️

Chemical Structure Depiction

⏏

O

O



+

-

[▶ PubChem](#)

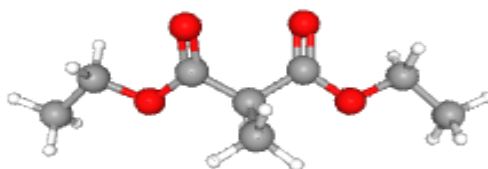
1.2 3D Conformer



Interactive Chemical Structure Model

☒ Ball and Stick ☐ Sticks ☐ Wire-Frame ☐ Space-Filling

☒ Show Hydrogens ☐ Animate



+

-



Conformer 1

of 10

[▶ PubChem](#)

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



diethyl 2-methylpropanedioate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.2 InChI



InChI=1S/C₈H₁₄O₄/c1-4-11-7(9)6(3)8(10)12-5-2/h6H,4-5H₂,1-3H₃

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.3 InChIKey



UPQZOUHVTJNGFK-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

► [PubChem](#)

2.1.4 SMILES



CCOC(=O)C(C)C(=O)OCC

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

► [PubChem](#)

2.2 Molecular Formula



C₈H₁₄O₄

Computed by PubChem 2.2 (PubChem release 2021.10.14)

► [Australian Industrial Chemicals Introduction Scheme \(AICIS\)](#); [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



609-08-5

- ▶ Australian Industrial Chemicals Introduction Scheme (AICIS); CAS Common Chemistry; ChemID...

2.3.2 Deprecated CAS



141885-94-1, 581796-71-6

- ▶ ChemIDplus; EPA Chemicals under the TSCA

581796-71-6

- ▶ EPA DSSTox

2.3.3 European Community (EC) Number



210-175-7

- ▶ European Chemicals Agency (ECHA)

2.3.4 UNII



7KD9S8CQN2

- ▶ FDA Global Substance Registration System (GSRS)

2.3.5 DSSTox Substance ID



DTXSID0060565

- ▶ EPA DSSTox

2.3.6 Nikkaji Number



J43.453A

- ▶ Japan Chemical Substance Dictionary (Nikkaji)

2.3.7 NSC Number



8700

[▶ DTP/NCI](#)

2.3.8 Wikidata



Q63395288

[▶ Wikidata](#)

2.4 Synonyms



2.4.1 Depositor-Supplied Synonyms



DIETHYL METHYLMALONATE	7KD9S8CQN2
609-08-5	2-Methylmalonic acid diethyl ester
Diethyl 2-methylmalonate	NSC-8700
diethyl 2-methylpropanedioate	Propanedioic acid, 2-methyl-, 1,3-diethyl ester
Methylmalonic acid diethyl ester	2-methyl-propanedioic acid diethyl ester
1,3-diethyl 2-methylpropanedioate	DIETHYLMETHYLMALONATE
Propanedioic acid, methyl-, diethyl ester	Ethyl methylmalonate (VAN)
Malonic acid, methyl-, diethyl ester	2-Methylmalonic acid diethyl
diethyl methylpropanedioate	2-Methylpropanedioic Acid 1,3-Diethyl Ester; Methylmalonic
Ethyl methylmalonate	Methylmalonate; Diethyl Methylpropanedioate; Diethyl alpha

[▶ PubChem](#)

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name
Molecular Weight
Property Value
174.19 g/mol
Reference
Computed by PubChem 2.2 (PubChem release 2021.10.14)
Property Name
XLogP3-AA

Property Value

1.4

Reference

Computed by XLogP3 3.0 (PubChem release 2021.10.14)

Property Name

Hydrogen Bond Donor Count

Property Value

0

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Hydrogen Bond Acceptor Count

Property Value

4

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Rotatable Bond Count

Property Value

6

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Exact Mass

Property Value

174.08920892 g/mol

Reference

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name

Monoisotopic Mass

Property Value

174.08920892 g/mol

Reference

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name

Topological Polar Surface Area

Property Value

52.6Å²

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Heavy Atom Count

Property Value

12

Reference

Computed by PubChem

Property Name

Formal Charge

Property Value

0

Reference

Computed by PubChem

Property Name

Complexity

Property Value

146

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Isotope Atom Count

Property Value

0

Reference

Computed by PubChem

Property Name

Defined Atom Stereocenter Count

Property Value

0

Reference

Computed by PubChem

Property Name

Undefined Atom Stereocenter Count

Property Value

0

Reference

Computed by PubChem

Property Name

Defined Bond Stereocenter Count

Property Value

0

Reference

Computed by PubChem

Property Name

Undefined Bond Stereocenter Count

Property Value

0

Reference

Computed by PubChem

Property Name

Covalently-Bonded Unit Count

Property Value

1

Reference

Computed by PubChem

Property Name

Compound Is Canonicalized

Property Value

Yes

Reference

Computed by PubChem (release 2021.10.14)

► [PubChem](#)

3.2 Experimental Properties



3.2.1 Physical Description



Clear colorless liquid; [Acros Organics MSDS]

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

3.2.2 Kovats Retention Index



Standard non-polar
1073

Standard polar
1539

► [NIST Mass Spectrometry Data Center](#)

3.3 SpringerMaterials Properties



[Boiling point](#)
[Density](#)
[Heat of sublimation](#)
[Optical coefficient](#)
[Refractive index](#)
[Surface tension](#)
[Thermal expansion coefficient](#)
[Vapor pressure](#)

► [SpringerMaterials](#)

3.4 Chemical Classes



Other Classes -> Esters, Other

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

4 Spectral Information



4.1 1D NMR Spectra



1D NMR Spectra
[NMRShiftDB Link](#)

► [NMRShiftDB](#)

4.1.1 1H NMR Spectra

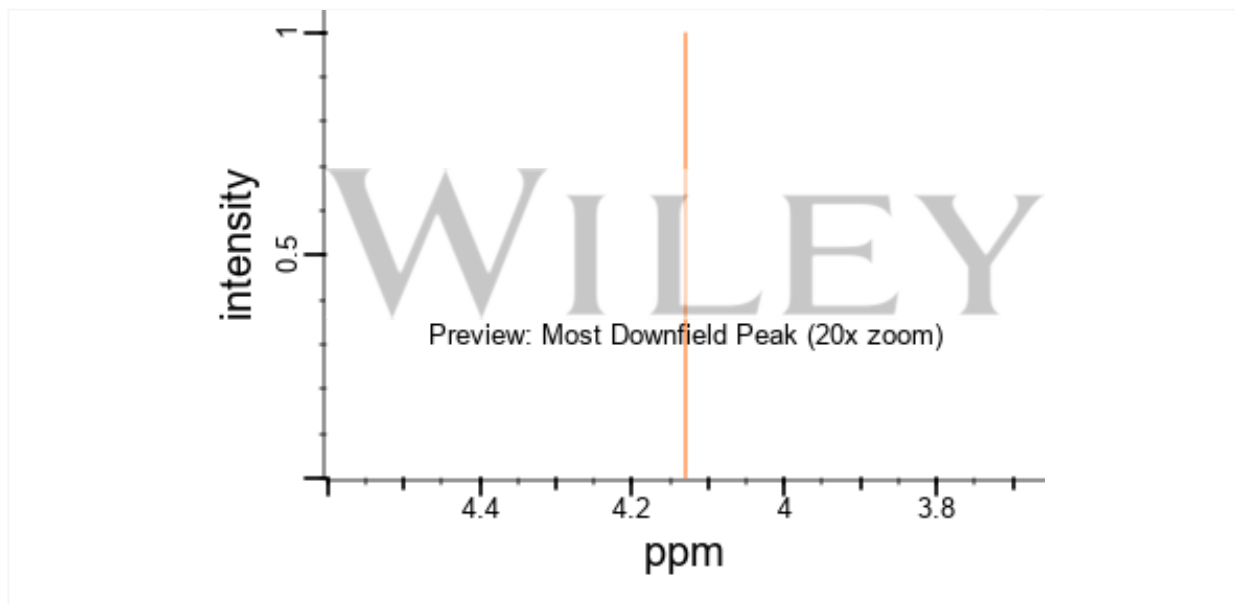


1 of 2

Instrument Name
Varian A-60D

Copyright
Copyright © 2009-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



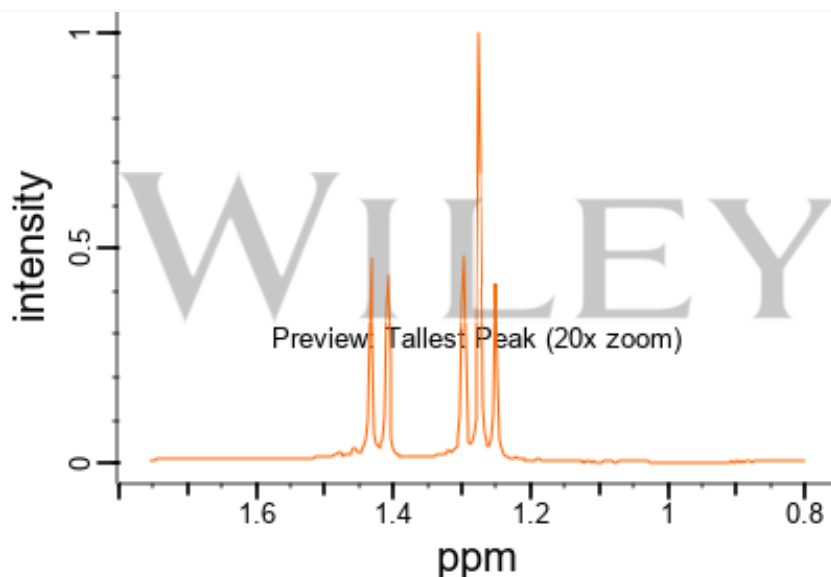
► [SpectraBase](#)

2 of 2

Instrument Name
Bruker WH-300

Copyright
Copyright © 2002-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.

Thumbnail



► SpectraBase

4.1.2 ¹³C NMR Spectra



1 of 2

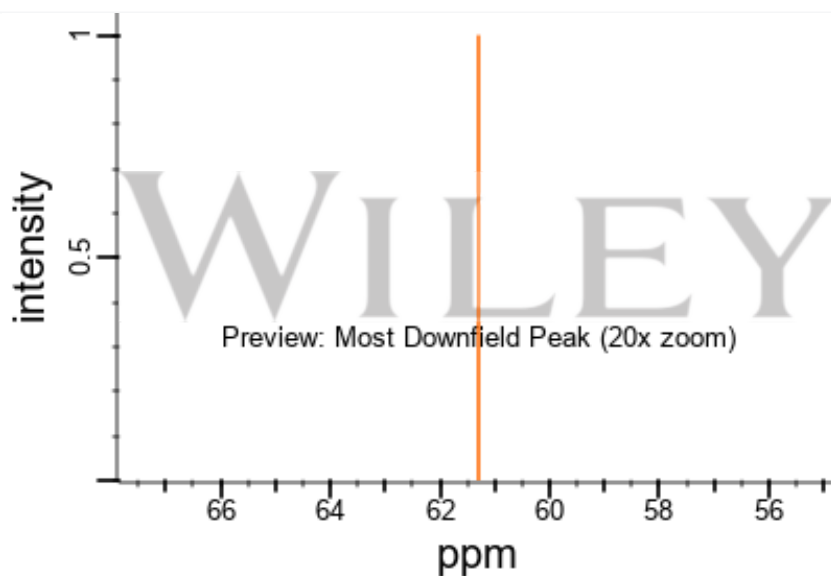
Source of Sample

Aldrich Chemical Company, Inc., Milwaukee, Wisconsin

Copyright

Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



► SpectraBase

2 of 2

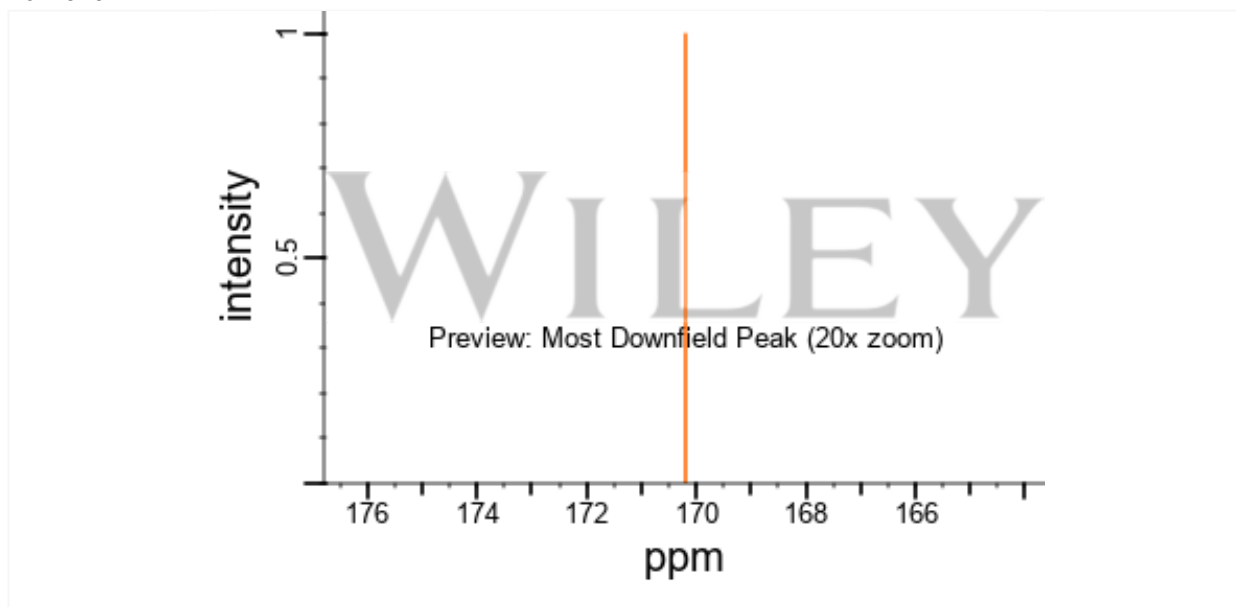
Instrument Name

Varian HA-100

Copyright

Copyright © 2002-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.

Thumbnail

[► SpectraBase](#)

4.2 Mass Spectrometry



4.2.1 GC-MS



1 of 6

[View All](#)

MoNA ID

[JP009794](#)

MS Category

Experimental

MS Type

GC-MS

MS Level

MS1

Instrument

JEOL JMS-D-300

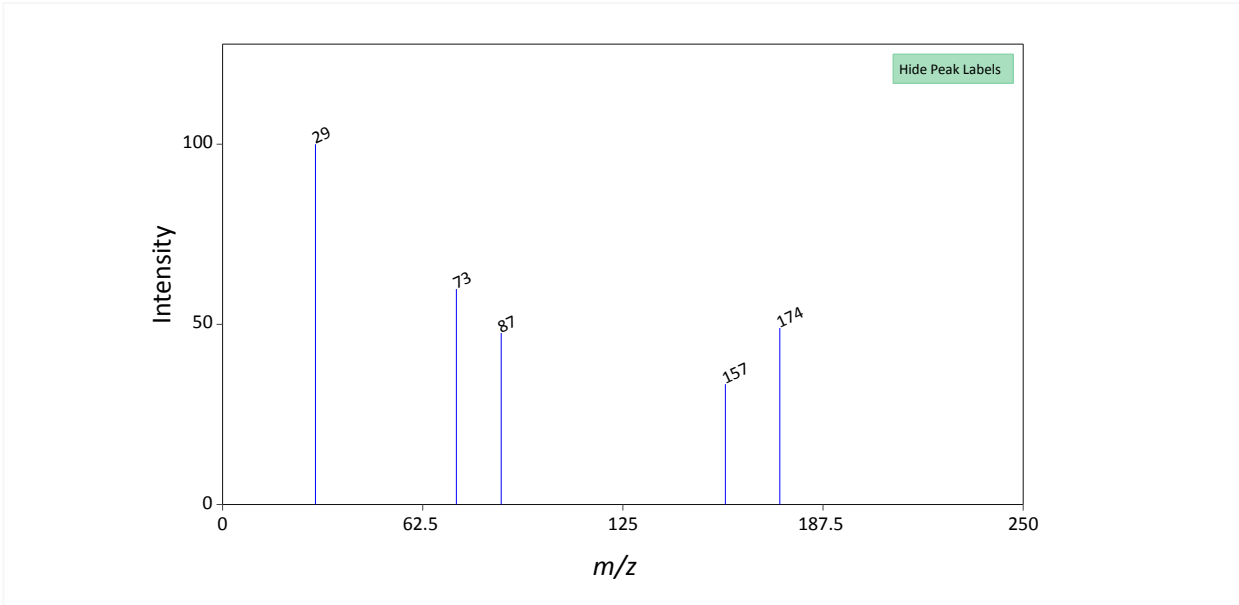
Instrument Type
EI-B

Ionization Mode
positive

Top 5 Peaks
29 99.99
73 59.80
174 49
87 47.60
157 33.40

SPLASH
[splash10-05i0-9500000000-76e1858b1ac18b781fc5](#)

Thumbnail



License
CC BY-NC-SA

► [MassBank of North America \(MoNA\)](#)

2 of 6

View All

NIST Number
229807

Library
Main library

Total Peaks

59

m/z Top Peak

29

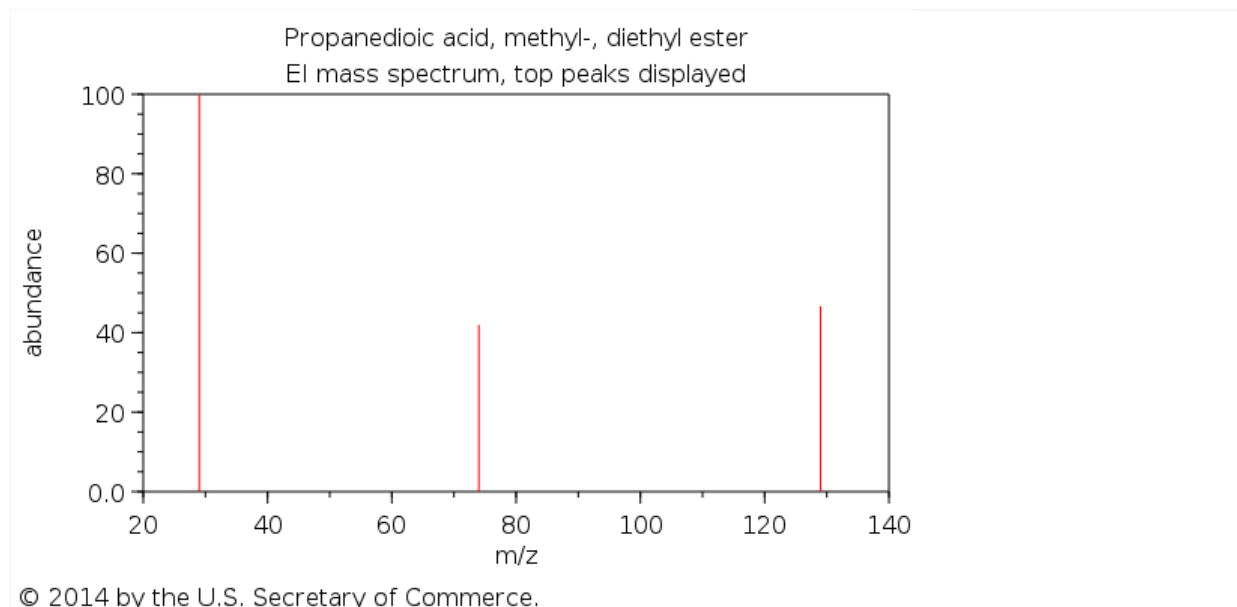
m/z 2nd Highest

129

m/z 3rd Highest

74

Thumbnail

[► NIST Mass Spectrometry Data Center](#)

4.2.2 Other MS



Accession ID

[MSBNK-Fac_Eng_Univ_Tokyo-JP009794](#)

Authors

KURARAY CO., LTD.

Instrument

JEOL JMS-D-300

Instrument Type

EI-B

MS Level

MS

Ionization Mode
POSITIVEIonization
ENERGY 70 eV

Top 5 Peaks

29 999

73 598

174 490

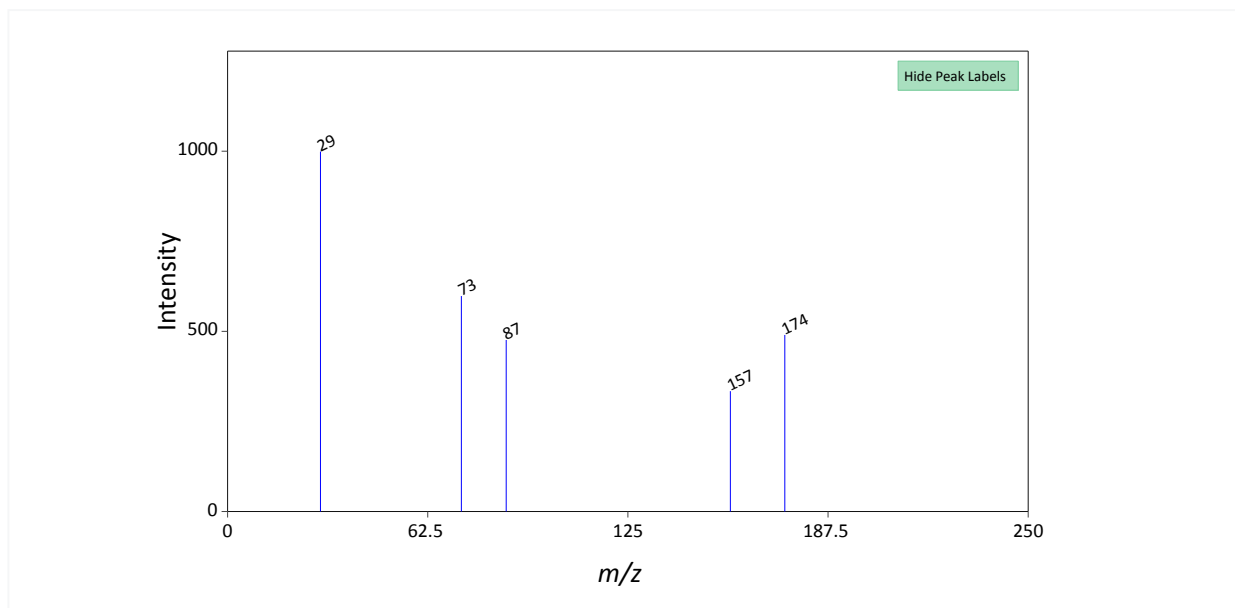
87 476

157 334

SPLASH

[splash10-05i0-9500000000-76e1858b1ac18b781fc5](#)

Thumbnail



License

CC BY-NC-SA

[► MassBank Europe](#)

4.3 IR Spectra



4.3.1 FTIR Spectra



1 of 2

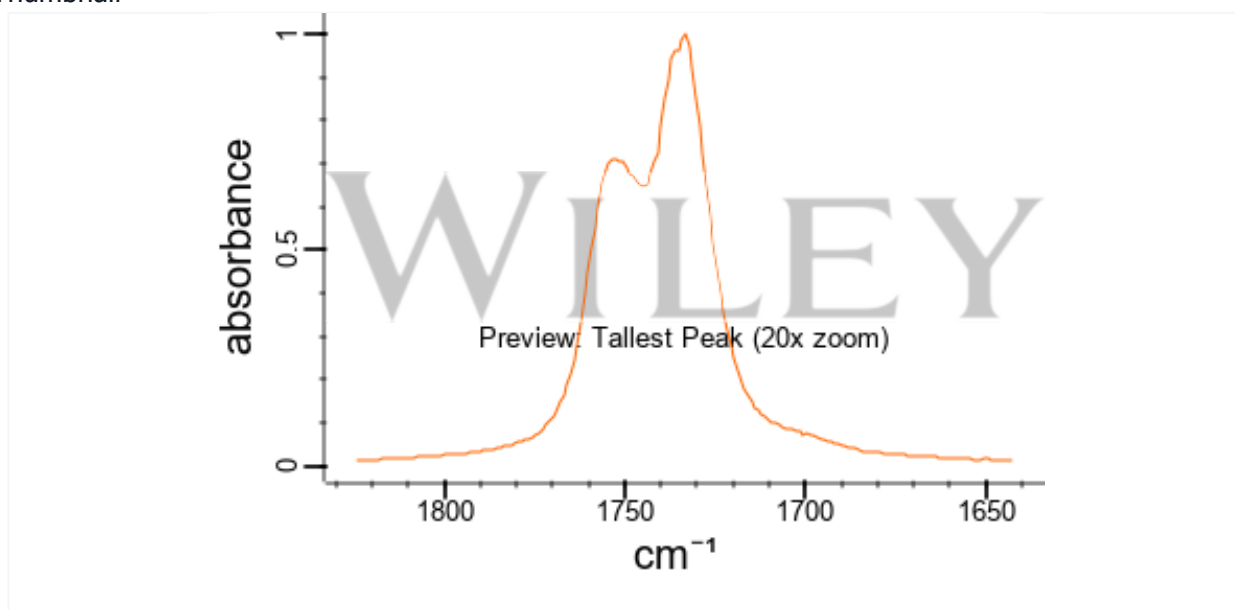
Instrument Name
Bio-Rad FTS

Technique
Neat (KBr)

Source of Spectrum
Forensic Spectral Research

Copyright
Copyright © 2012-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



► [SpectraBase](#)

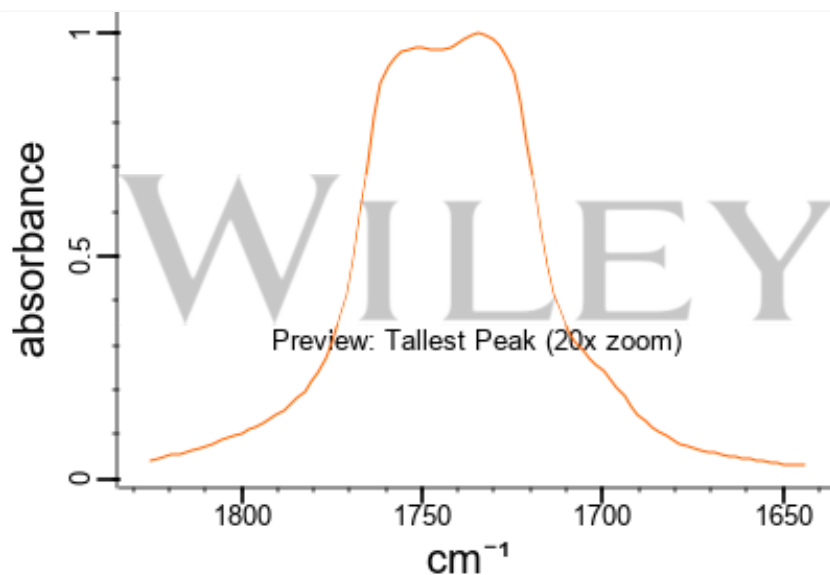
2 of 2

Instrument Name
Bruker IFS 85

Technique
Film

Copyright
Copyright © 1989, 1990-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.

Thumbnail



► SpectraBase

4.3.2 ATR-IR Spectra



1 of 2

Instrument Name

PerkinElmer SpectrumTwo

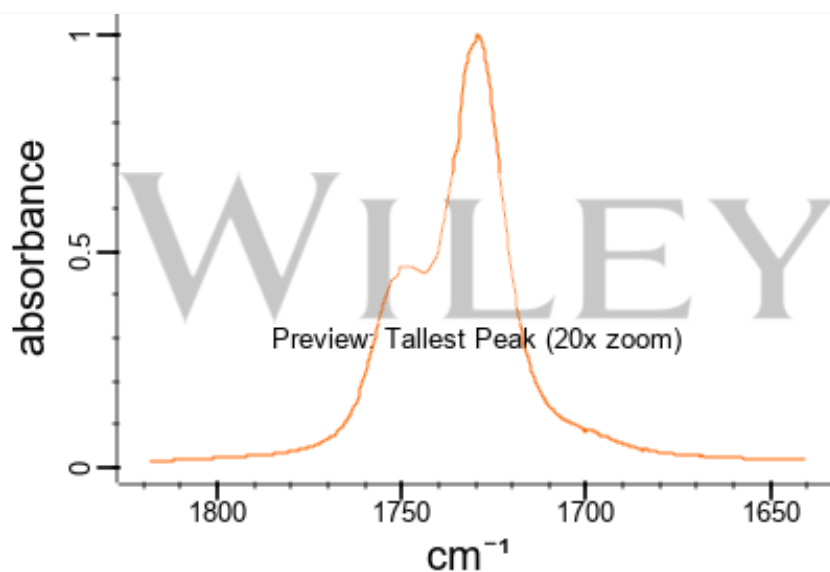
Technique

ATR-IR

Copyright

Copyright © 2012-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



[▶ SpectraBase](#)

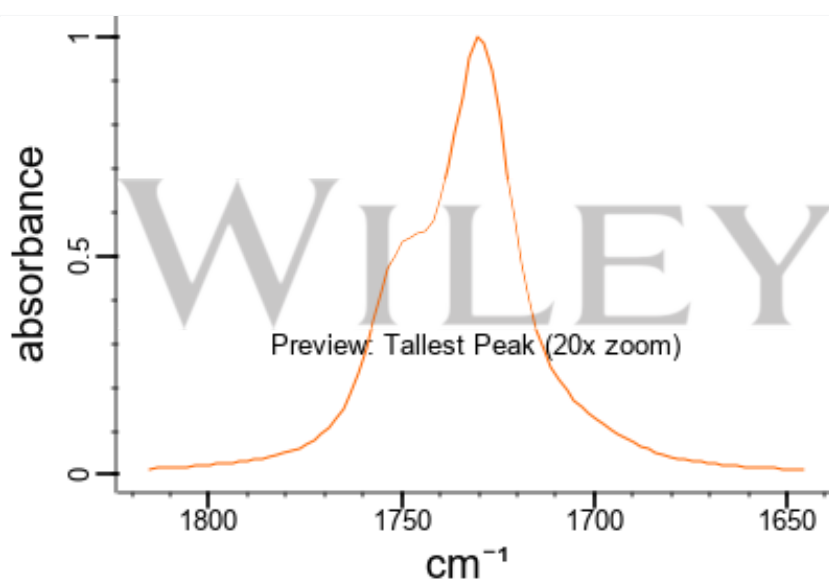
2 of 2

Source of Sample
Aldrich

Catalog Number
126136

Copyright
Copyright © 2018-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2018-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

[▶ SpectraBase](#)

4.3.3 Near IR Spectra



1 of 2

Instrument Name
BRUKER IFS 88

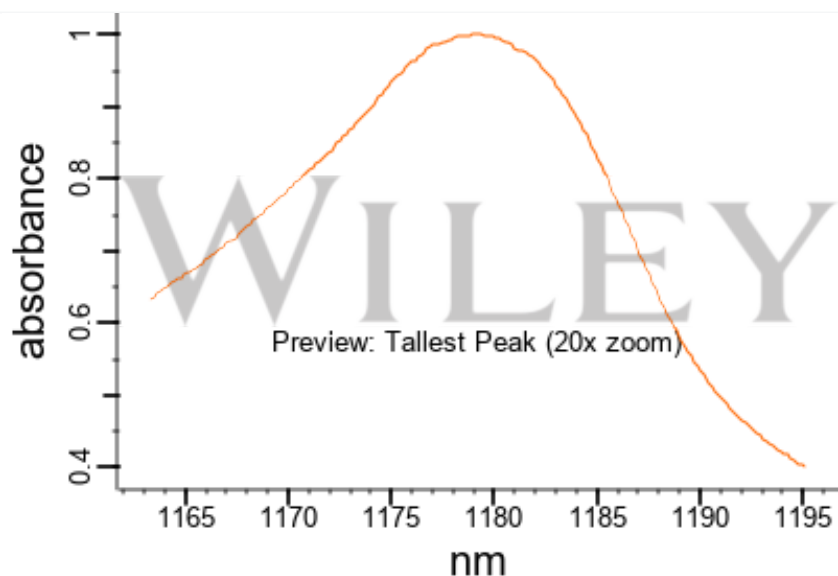
Technique
NIR Spectrometer= INSTRUMENT
PARAMETERS=INST=BRUKER,RSN=7158,REO=2,CNM=HEI,ZFF=2

Source of Spectrum
Prof. Buback, University of Goettingen, Germany

Copyright

Copyright © 1989, 1990-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.

Thumbnail



► SpectraBase

2 of 2

Instrument Name

BRUKER IFS 88

Technique

NIR Spectrometer= INSTRUMENT

PARAMETERS=INST=BRUKER,RSN=7158,REO=2,CNM=HEI,ZFF=2

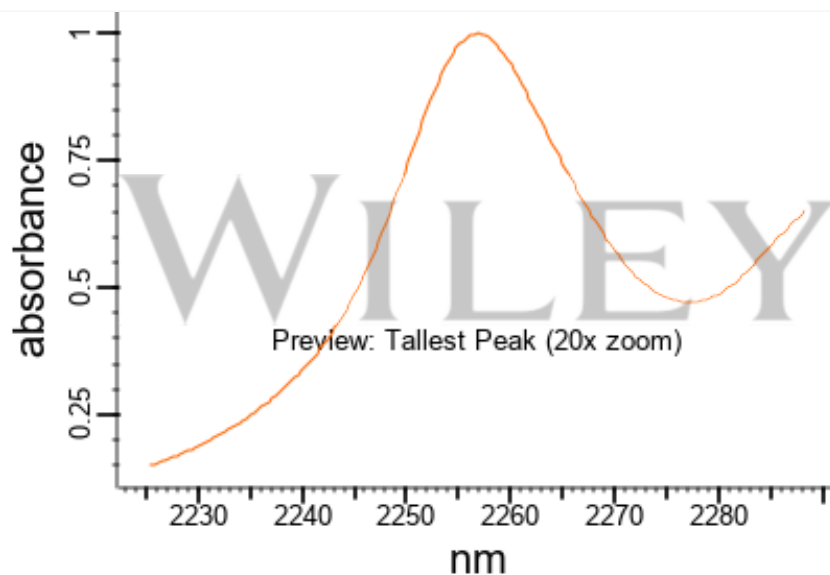
Source of Spectrum

Prof. Buback, University of Goettingen, Germany

Copyright

Copyright © 1989, 1990-2024 Wiley-VCH Verlag GmbH & Co. KGaA. All Rights Reserved.

Thumbnail



► SpectraBase

4.3.4 Vapor Phase IR Spectra



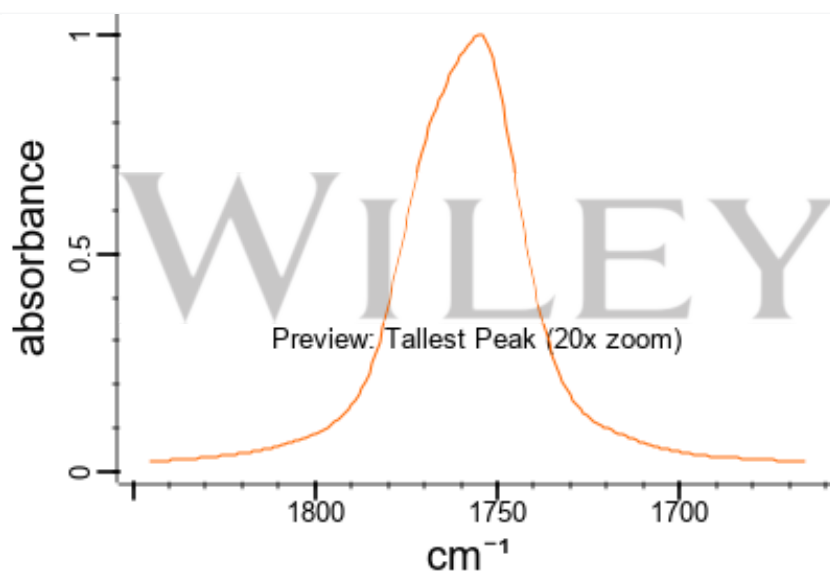
1 of 2

Instrument Name
DIGILAB FTS-14

Technique
Vapor Phase

Copyright
Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



[▶ SpectraBase](#)

2 of 2

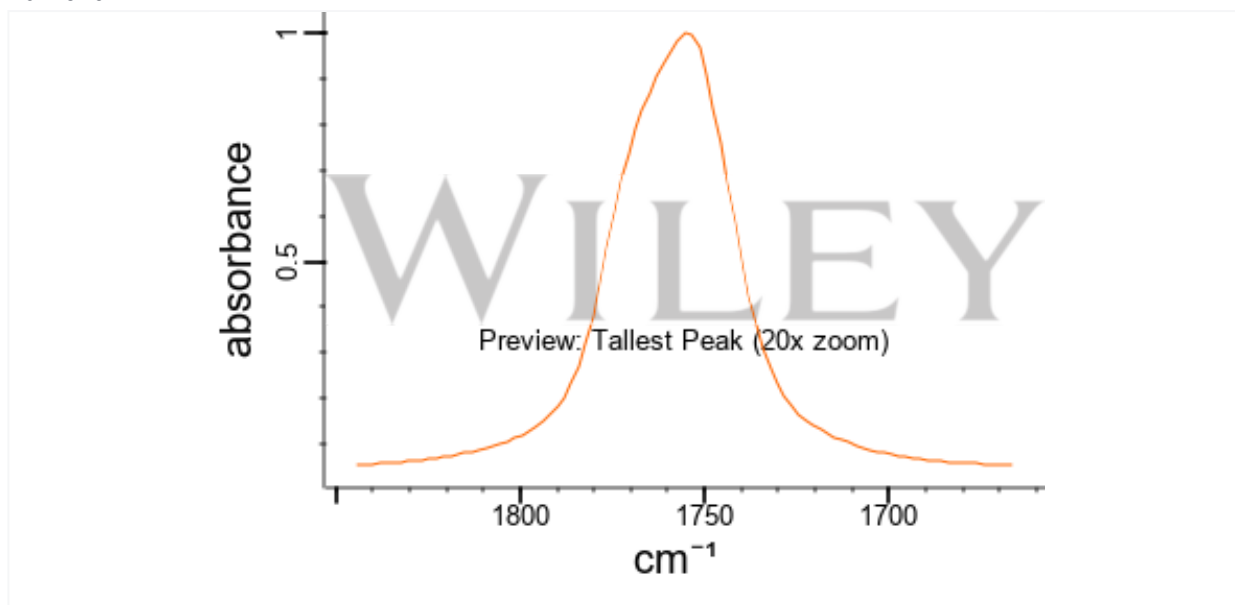
Source of Spectrum
Sigma-Aldrich Co. LLC.

Source of Sample
Sigma-Aldrich Co. LLC.

Catalog Number
126136

Copyright
Copyright © 2021-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2021 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail

[▶ SpectraBase](#)

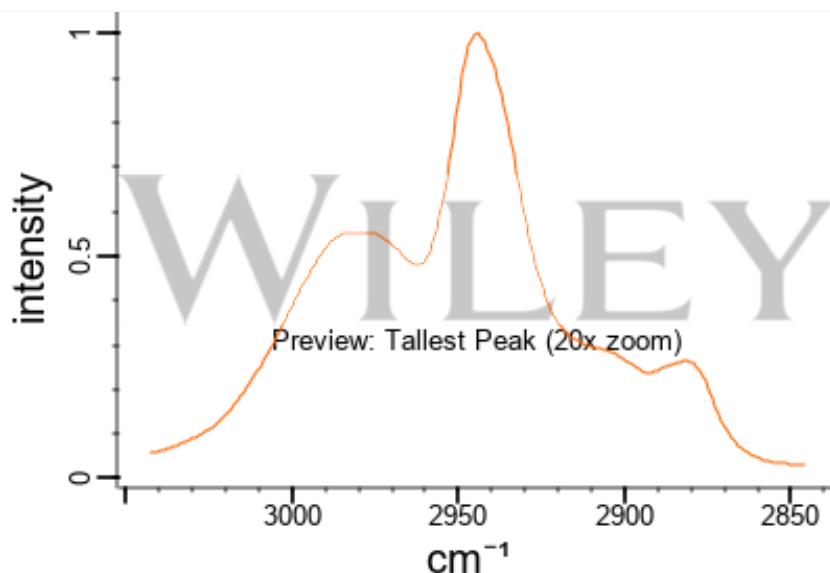
4.4 Raman Spectra



Catalog Number
126136

Copyright
Copyright © 2017-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2017-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



► [SpectraBase](#)

5 Related Records



5.1 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](#)

5.2 Related Compounds



Same Connectivity Count

[3](#)

Same Parent, Connectivity Count

[15](#)

Same Parent, Exact Count

[13](#)

Mixtures, Components, and Neutralized Forms Count

[133](#)

Similar Compounds (2D)

[View in PubChem Search](#)

Similar Conformers (3D)
[View in PubChem Search](#)

► [PubChem](#)

5.3 Substances



5.3.1 Related Substances



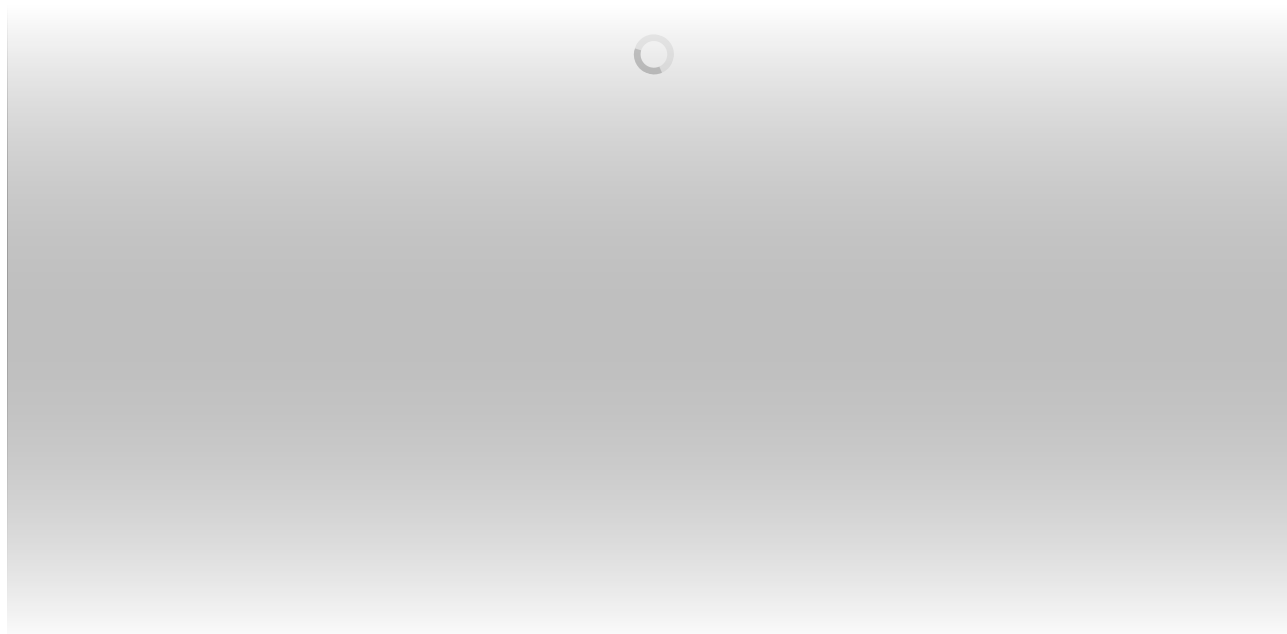
All Count
[315](#)

Same Count
[166](#)

Mixture Count
[149](#)

► [PubChem](#)

5.3.2 Substances by Category



► [PubChem](#)

5.4 Entrez Crosslinks

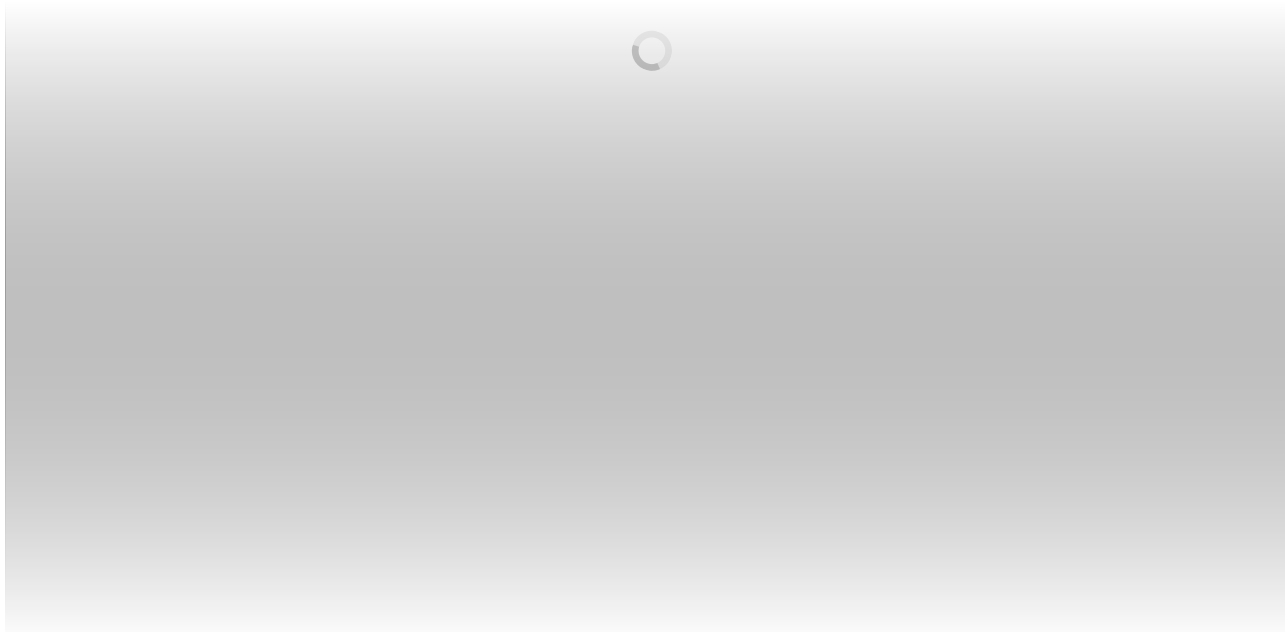


PubMed Count

8

[▶ PubChem](#)

6 Chemical Vendors

[▶ PubChem](#)

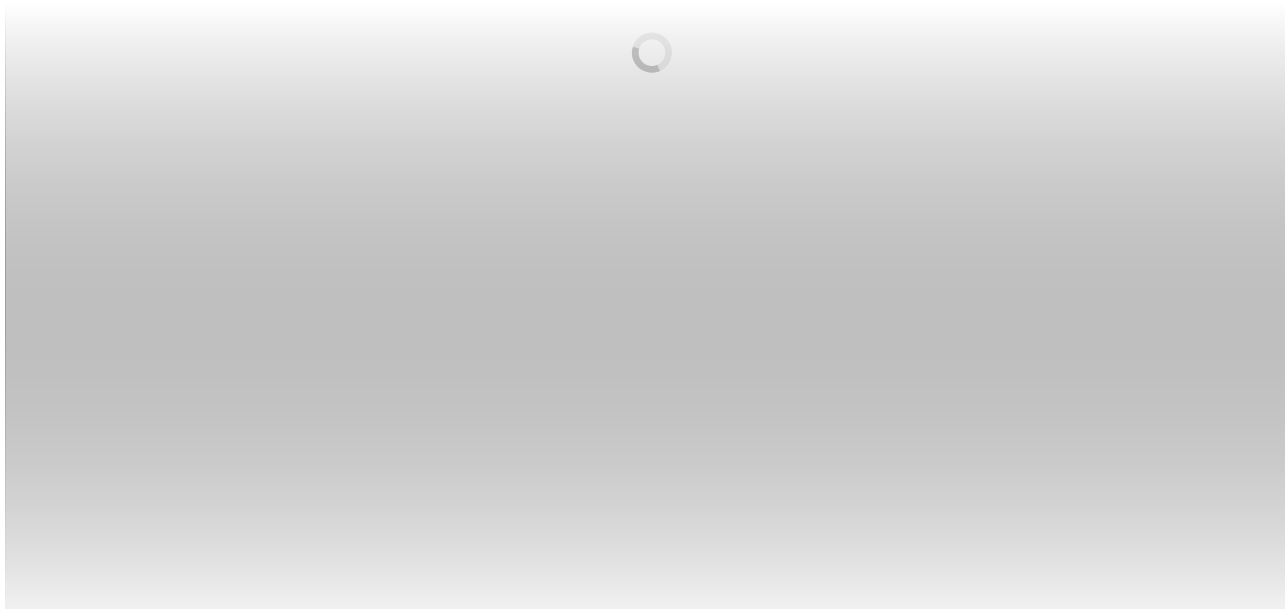
7 Use and Manufacturing



7.1 Uses



EPA CPDat Chemical and Product Categories



The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), DOI:10.1038/sdata.2018.125

► [EPA Chemical and Products Database \(CPDat\)](#)

7.2 General Manufacturing Information



EPA TSCA Commercial Activity Status

[Propanedioic acid, 2-methyl-, 1,3-diethyl ester](#): ACTIVE

► [EPA Chemicals under the TSCA](#)

8 Safety and Hazards



8.1 Hazards Identification



8.1.1 GHS Classification



Note

This chemical does not meet GHS hazard criteria for 75% (6 of 8) of all reports. Pictograms displayed are for 25% (2 of 8) of reports that indicate hazard statements.

Pictogram(s)



Irritant

Signal

Warning

GHS Hazard Statements

H315 (25%): Causes skin irritation [[Warning](#) Skin corrosion/irritation]

H319 (25%): Causes serious eye irritation [[Warning](#) Serious eye damage/eye irritation]

H335 (25%): May cause respiratory irritation [[Warning](#) Specific target organ toxicity, single exposure; Respiratory tract irritation]

Precautionary Statement Codes

P261, P264, P264+P265, P271, P280, P302+P352, P304+P340, P305+P351+P338, P319, P321, P332+P317, P337+P317, P362+P364, P403+P233, P405, 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 8 reports by companies from 3 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.

Reported as not meeting GHS hazard criteria per 6 of 8 reports by companies. For more detailed information, please visit [ECHA C&L website](#).

There is 1 notification provided by 2 of 8 reports by companies with hazard statement code(s).

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 \(ECHA\)](#)

8.1.2 Hazard Classes and Categories



Skin Irrit. 2 (25%)

Eye Irrit. 2A (25%)

STOT SE 3 (25%)

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

8.1.3 Hazards Summary



May cause irritation; [Acros Organics MSDS] See [Malonic acid](#).

► [Haz-Map, Information on Hazardous Chemicals and Occupational Diseases](#)

8.2 Regulatory Information



The Australian Inventory of Industrial Chemicals

Chemical: [Propanedioic acid](#), methyl-, diethyl ester

► [Australian Industrial Chemicals Introduction Scheme \(AICIS\)](#)

REACH Registered Substance

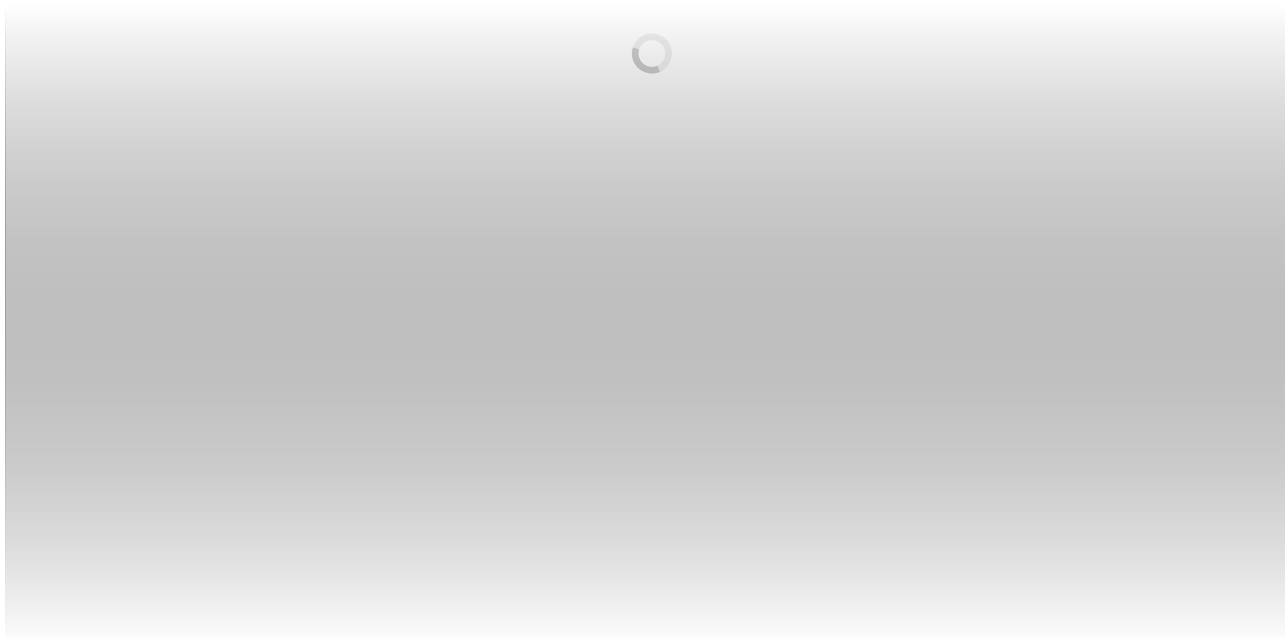
Status: Active Update: 13-03-2018 <https://echa.europa.eu/registration-dossier/-/registered-dossier/18586>

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

9 Literature

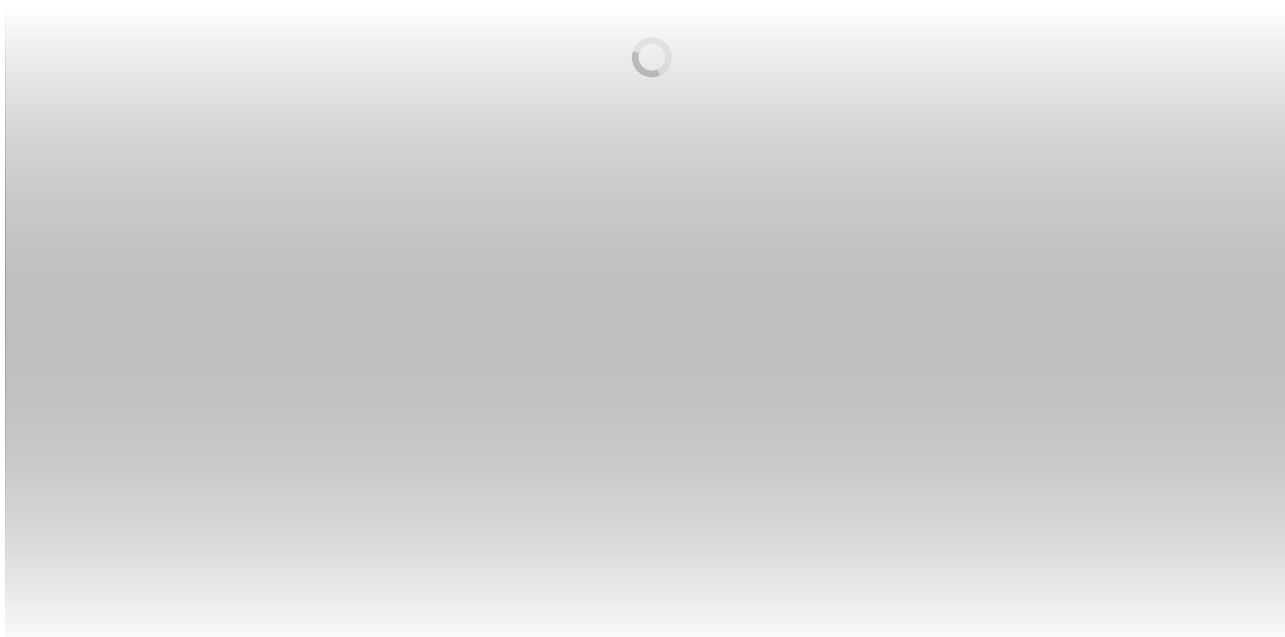


9.1 Consolidated References



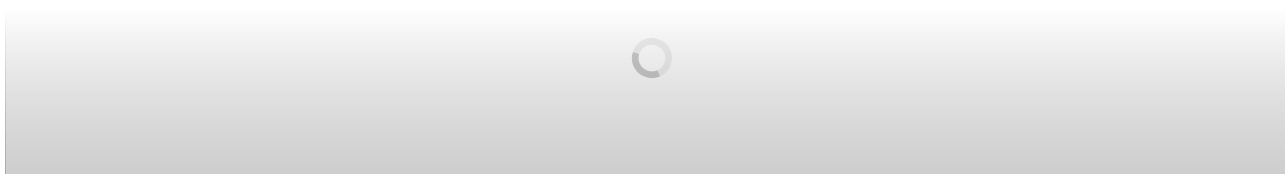
► PubChem

9.2 Springer Nature References



► Springer Nature

9.3 Thieme References



► Thieme Chemistry

9.4 Wiley References



► Wiley

9.5 Nature Journal References



Li et al. Organo-metal cooperative catalysis for C(sp³)-H alkylation polymerization. Nature Synthesis, DOI: 10.1038/s44160-023-00389-1, published online 7 September 2023

► Nature Synthesis

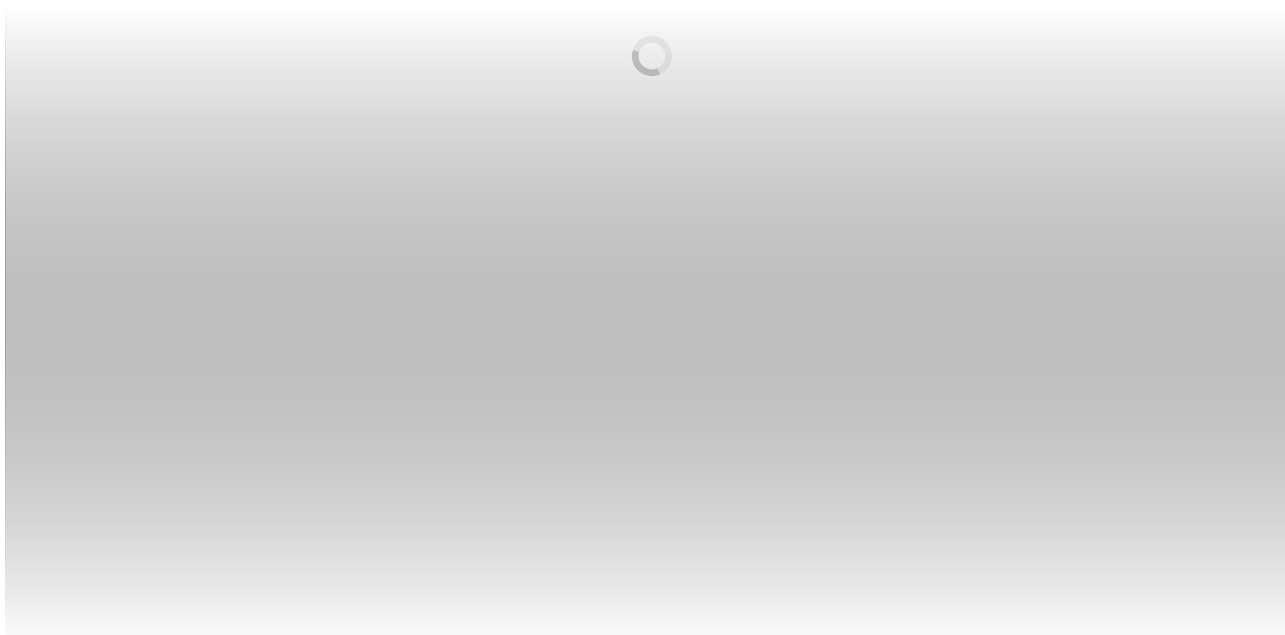
9.6 Chemical Co-Occurrences in Literature





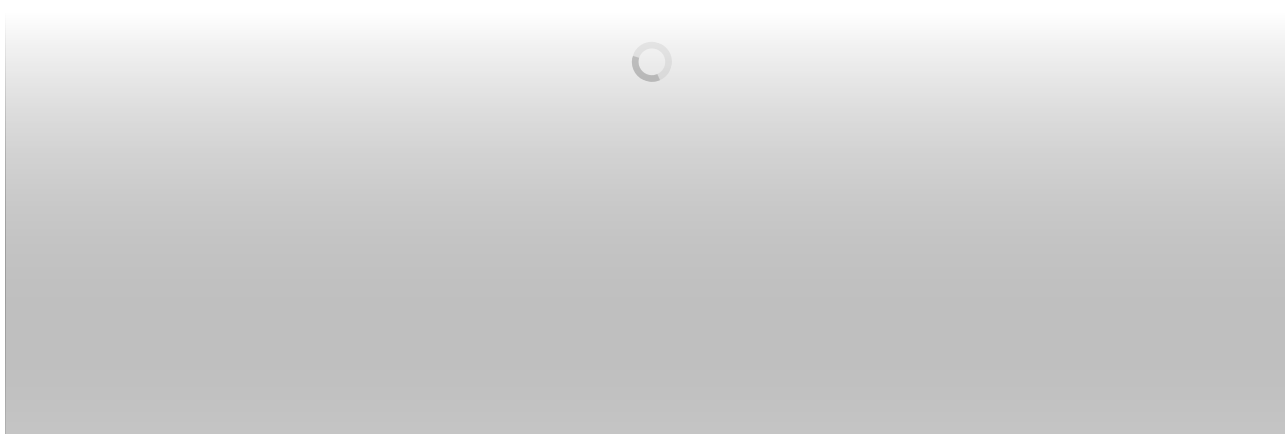
► PubChem

9.7 Chemical-Gene Co-Occurrences in Literature



► PubChem

9.8 Chemical-Disease Co-Occurrences in Literature



[▶ PubChem](#)

10 Patents



10.1 Depositor-Supplied Patent Identifiers



3,749 items



SORT BY Priority Date - Most Recent

[Aqueous coating composition for corrosion protection](#)Publication Number: [WO-2022229174-A1](#)

Priority Date: 2021-04-27

[Isoindolinone amide compounds useful to treat diseases associated with gspt1](#)Publication Number: [WO-202219412-A1](#)

Priority Date: 2021-04-14

[Pharmaceutical compositions for use in the prevention and treatment of a disease or disorder caused by or associated with one or more premature termination codons](#)Publication Number: [WO-202200857-A1](#)

Priority Date: 2021-03-22

[Isoindolinone compounds](#)Publication Number: [WO-2022152821-A1](#)

Priority Date: 2021-01-13

[Heterocyclic spiro compounds and methods of use](#)Publication Number: [WO-2022083569-A1](#)

Priority Date: 2020-10-20

<< < Page 1 of 750 > >>

[▶ PubChem](#)[Link to all deposited patent identifiers](#)

[▶ PubChem](#)

10.2 WIPO PATENTSCOPE



Patents are available for this chemical structure:

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

[▶ PATENTSCOPE \(WIPO\)](#)

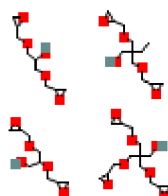
10.3 Chemical Co-Occurrences in Patents



Showing 3 of 100 [View More](#)



Chemical



[2,2-Bis\(oxiran-2-ylmethoxymethyl\)butan-1-ol;1,3-bis\(oxiran-2-ylmethoxy\)propan-2-ol;2,3-bis\(oxiran-2-ylmethoxy\)propan-1-ol;3-\(oxiran-2-ylmethoxy\)-2,2-bis\(oxiran-2-ylmethoxymethyl\)propan-1-ol](#)

[CID 160419817](#)

Selected evidence

1 patent from 1 patent family

[View All](#)

[Crosslinkers for coating compounds](#)

US-10227504-B2; Grant Date: 2019-03-12

Chemical



[\(E\)-N-methoxybutan-2-imine](#)

[CID 14744526](#)

Selected evidence

1 patent from 1 patent family

[View All](#)

[Crosslinkers for coating compounds](#)

US-10227504-B2; Grant Date: 2019-03-12

Chemical



[1-Ethyl-1,3,3,5-tetramethylcyclohexane](#)

[CID 159947088](#)

Selected evidence

1 patent from 1 patent family

[View All](#)

[Crosslinkers for coating compounds](#)

US-10227504-B2; Grant Date: 2019-03-12

[► PubChem](#)

10.4 Chemical-Disease Co-Occurrences in Patents



Showing 3 of 100 [View More](#)



Disease

[Inflammation](#)

Selected evidence

18 patents from 13 patent families

[View All](#)

[Dopamine functionalized polyurethane as tissue adhesive and manufacturing as same](#)

KR-102392208-B1; Grant Date: 2022-04-27

[1,2-oxazinyl phenyl alkanolic acids](#)

US-3586676-A; Grant Date: 1971-06-22

[1,2-oxazine derivatives in alleviating pain and treating inflammatory diseases](#)

US-3729559-A; Grant Date: 1973-04-24

Disease

[Foreign-Body Reaction](#)

Selected evidence

1 patent from 1 patent family

[View All](#) [Dopamine functionalized polyurethane as tissue adhesive and manufacturing as same](#)

KR-102392208-B1; Grant Date: 2022-04-27

Disease

[Platelet Aggregation, Spontaneous](#)

Selected evidence

5 patents from 4 patent families

[View All](#) [Thienothienylcarbonyl-phenylalkanoic acids and derivatives thereof](#)

US-4124596-A; Grant Date: 1978-11-07

[Thienothienylcarbonyl-phenylalkanoic acids and derivatives thereof](#)

US-4183944-A; Grant Date: 1980-01-15

[2-fluorophenylpropionic acid derivative](#)

KR-102071085-B1; Grant Date: 2020-01-29

[▶ PubChem](#)

10.5 Chemical-Gene Co-Occurrences in Patents

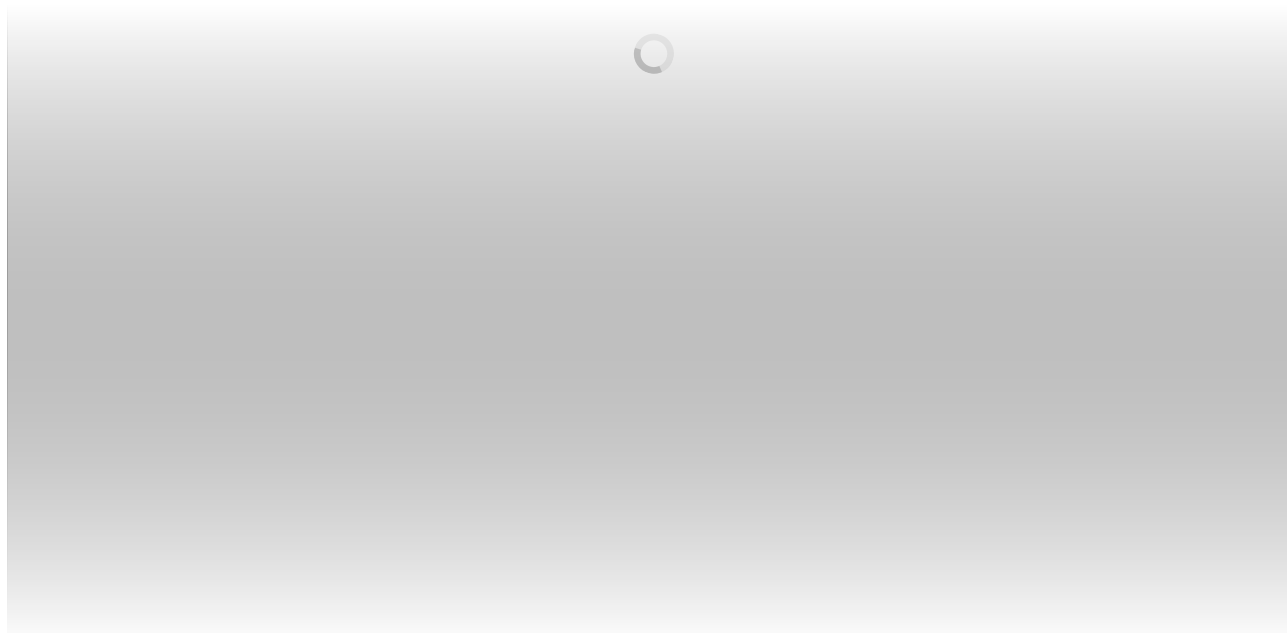


[▶ PubChem](#)

11 Biological Test Results



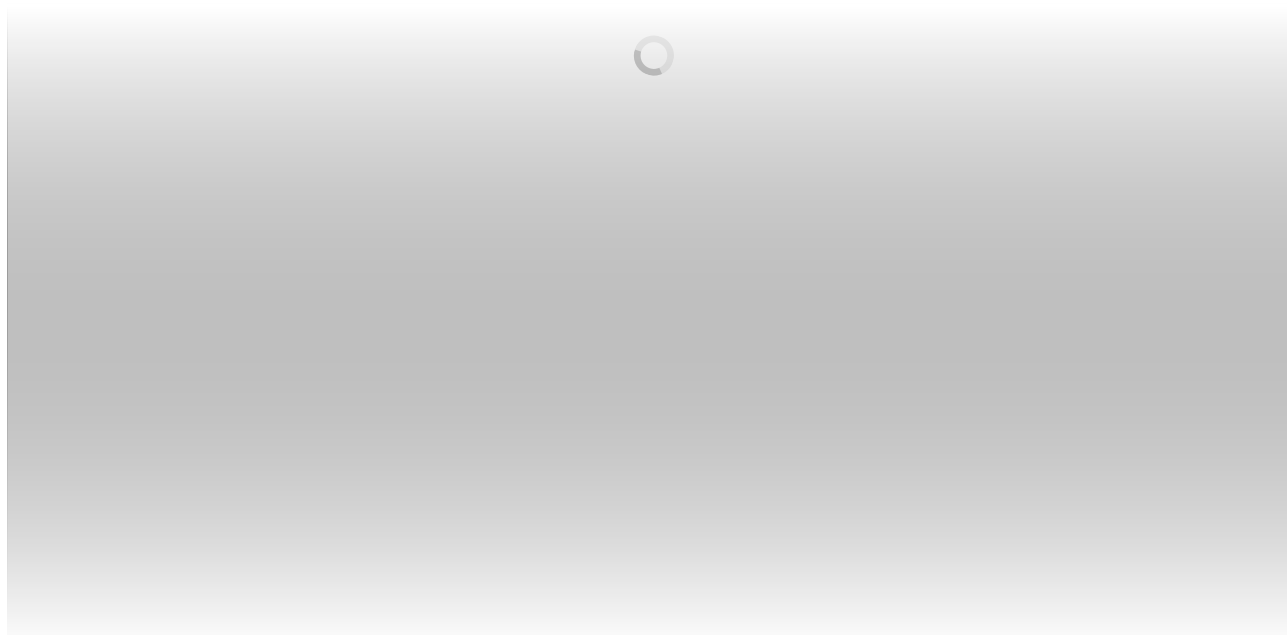
11.1 BioAssay Results

[▶ PubChem](#)

12 Classification

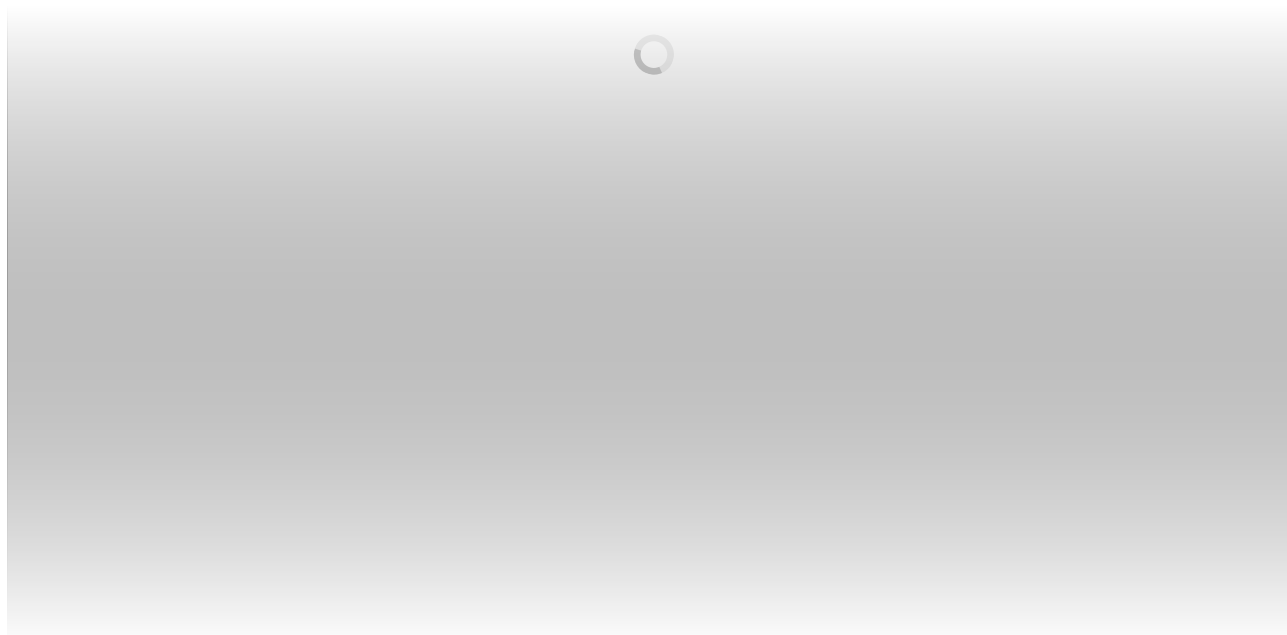


12.1 ChemIDplus

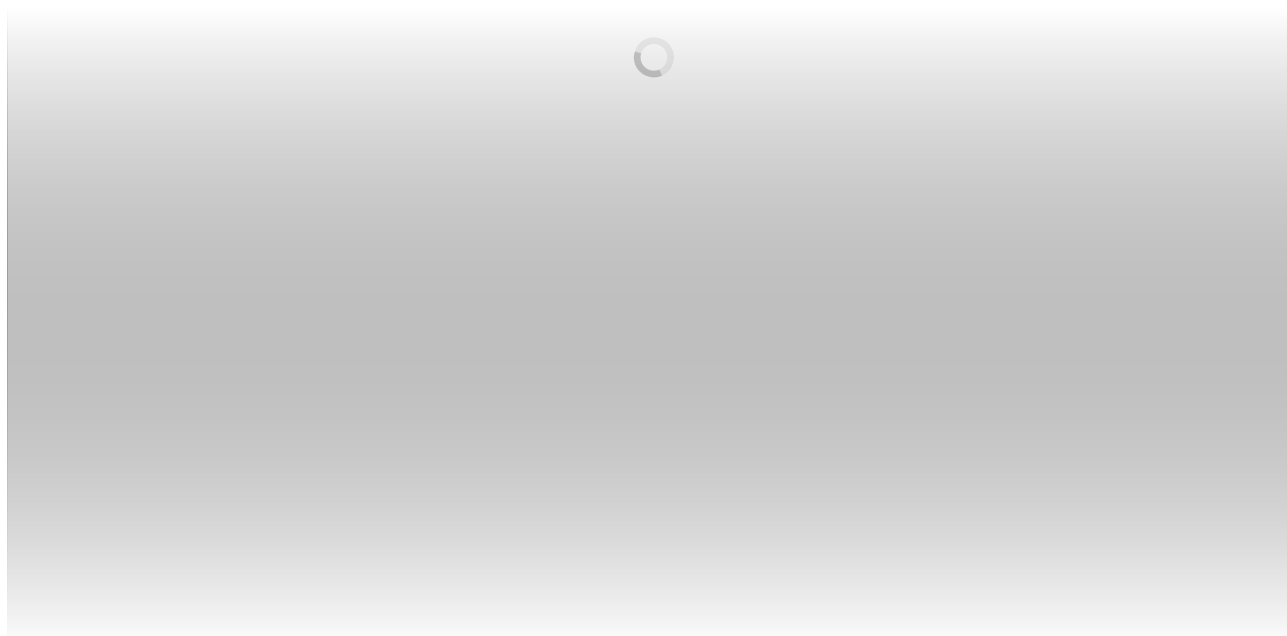


[▶ ChemIDplus](#)

12.2 UN GHS Classification

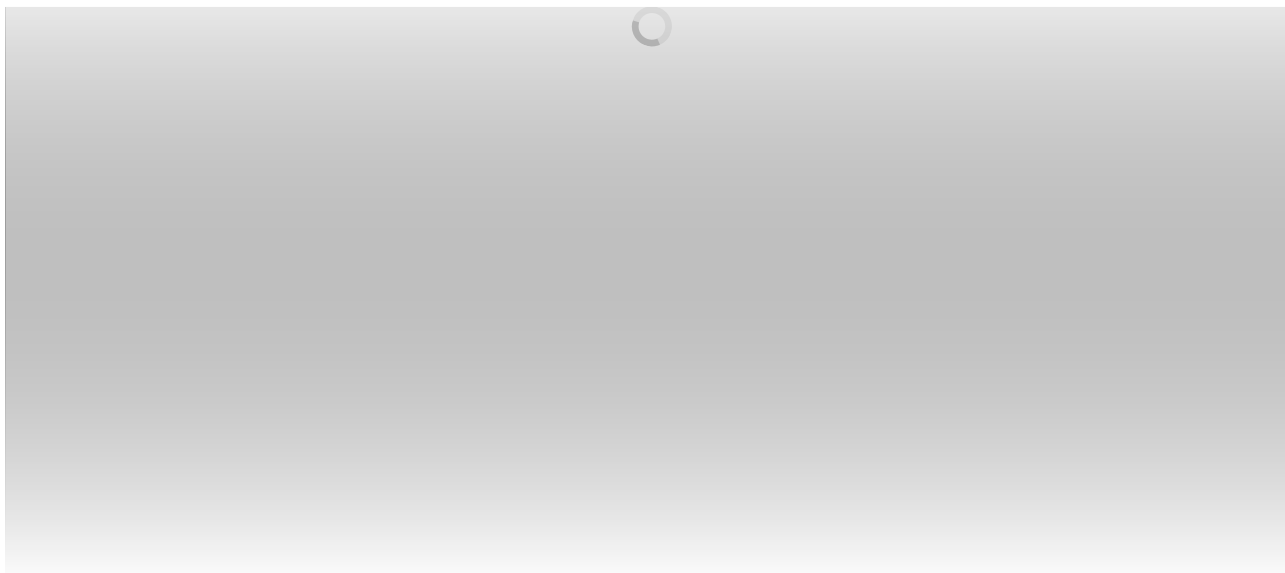
[▶ GHS Classification \(UNECE\)](#)

12.3 EPA CPDat Classification

[▶ EPA Chemical and Products Database \(CPDat\)](#)

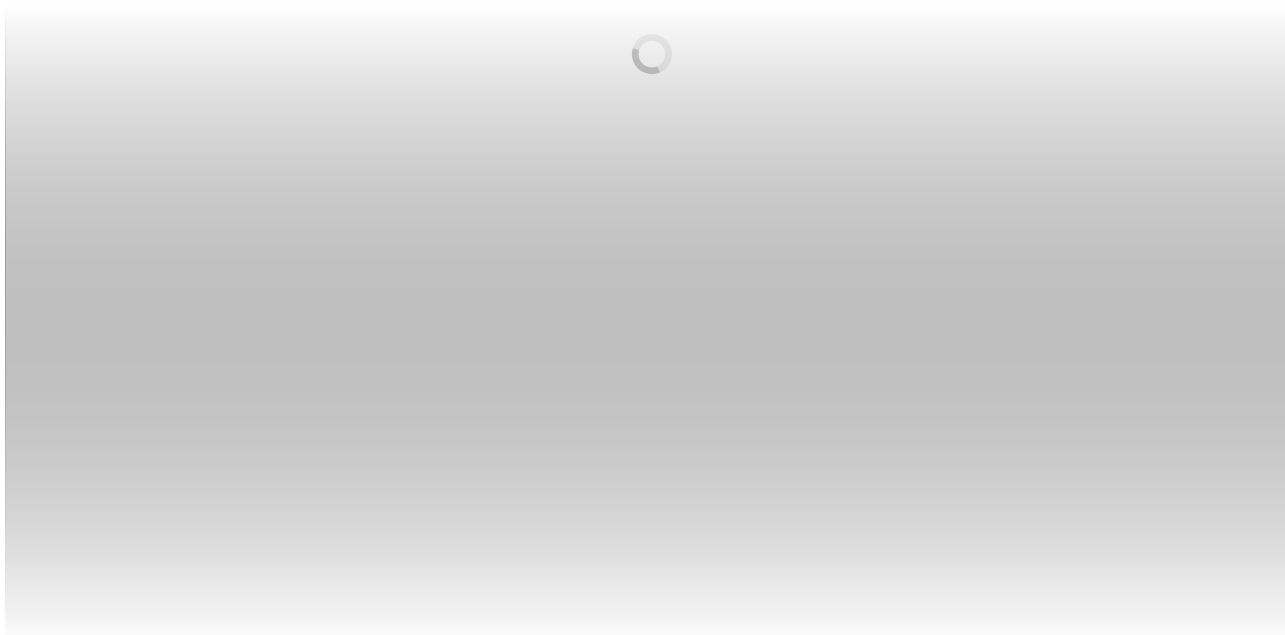
12.4 NORMAN Suspect List Exchange Classification





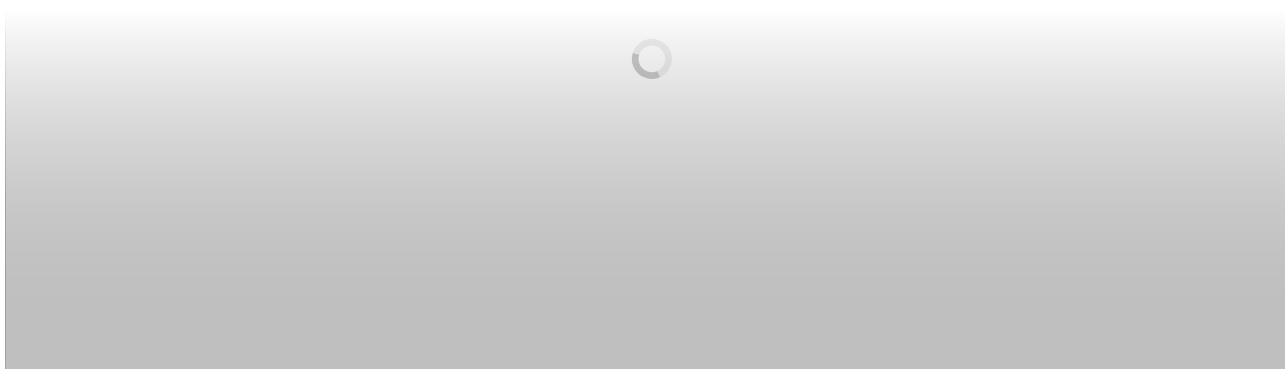
► NORMAN Suspect List Exchange

12.5 EPA DSSTox Classification



► EPA DSSTox

12.6 EPA TSCA and CDR Classification



► EPA Chemicals under the TSCA

12.7 EPA Substance Registry Services Tree



► EPA Substance Registry Services

13 Information Sources



FILTER BY SOURCE

ALL SOURCES



1. Australian Industrial Chemicals Introduction Scheme (AICIS)

LICENSE

<https://www.industrialchemicals.gov.au/copyright>

Propanedioic acid, methyl-, diethyl ester

<https://services.industrialchemicals.gov.au/search-inventory/>

2. CAS Common Chemistry

LICENSE

The data from CAS Common Chemistry is provided under a CC-BY-NC 4.0 license, unless otherwise stated.

<https://creativecommons.org/licenses/by-nc/4.0/>

Diethyl methylmalonate

https://commonchemistry.cas.org/detail?cas_rn=609-08-5

3. ChemIDplus

LICENSE

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

Diethyl methylmalonate

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0000609085>

ChemIDplus Chemical Information Classification

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

4. DTP/NCI

LICENSE

Unless otherwise indicated, all text within NCI products is free of copyright and may be reused without our permission. Credit the National Cancer Institute as the source.

<https://www.cancer.gov/policies/copyright-reuse>

DIETHYL METHYLMALONATE

<https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=8700>

5. EPA Chemicals under the TSCA

LICENSE

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

Propanedioic acid, 2-methyl-, 1,3-diethyl ester

<https://www.epa.gov/chemicals-under-tsca>

EPA TSCA Classification

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

6. EPA DSSTox

LICENSE

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

Propanedioic acid, methyl-, diethyl ester

<https://comptox.epa.gov/dashboard/DTXSID0060565>

CompTox Chemicals Dashboard Chemical Lists

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

7. European Chemicals Agency (ECHA)

LICENSE

Use of the information, documents and data from the ECHA website is subject to the terms and conditions of this Legal Notice, and subject to other binding limitations provided for under applicable law, the information, documents and data made available on the ECHA website may be reproduced, distributed and/or used, totally or in part, for non-commercial purposes provided that ECHA is acknowledged as the source: "Source: European Chemicals Agency, <http://echa.europa.eu/>". Such acknowledgement must be included in each copy of the material. ECHA permits and encourages organisations and individuals to create links to the ECHA website under the following cumulative conditions: Links can only be made to webpages that provide a link to the Legal Notice page.

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

Diethyl methylmalonate

<https://chem.echa.europa.eu/100.009.251>

Diethyl methylmalonate (EC: 210-175-7)<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/61298>8. **FDA Global Substance Registration System (GSRS)**

LICENSE

Unless otherwise noted, the contents of the FDA website (www.fda.gov), both text and graphics, are not copyrighted. They are in the public domain and may be republished, reprinted and otherwise used freely by anyone without the need to obtain permission from FDA. Credit to the U.S. Food and Drug Administration as the source is appreciated but not required.

<https://www.fda.gov/about-fda/about-website/website-policies#linking>*DIETHYL METHYLMALONATE*<https://gsrs.ncats.nih.gov/ginas/app/beta/substances/7KD9S8CQN2>9. **EPA Chemical and Products Database (CPDat)**

LICENSE

<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>*Propanedioic acid, methyl-, diethyl ester*<https://comptox.epa.gov/dashboard/DTXSID0060565#exposure>*EPA CPDat Classification*<https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat>10. **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

LICENSE

Copyright (c) 2022 Haz-Map(R). All rights reserved. Unless otherwise indicated, all materials from Haz-Map are copyrighted by Haz-Map(R). No part of these materials, either text or image may be used for any purpose other than for personal use. Therefore, reproduction, modification, storage in a retrieval system or retransmission, in any form or by any means, electronic, mechanical or otherwise, for reasons other than personal use, is strictly prohibited without prior written permission.

<https://haz-map.com/About>*Diethyl methylmalonate*<https://haz-map.com/Agents/20588>11. **Japan Chemical Substance Dictionary (Nikkaji)**http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J43.453A12. **MassBank Europe**

LICENSE

<https://github.com/MassBank/MassBank-web/blob/main/MassBank-Project/LICENSE.txt>*DIETHYL 2-METHYLPROPANEDIOATE*<https://massbank.eu/MassBank/Result.jsp?inchikey=UPQZOUHVTJNGFK-UHFFFAOYSA-N>13. **MassBank of North America (MoNA)**

LICENSE

The content of the MoNA database is licensed under CC BY 4.0.

<https://mona.fiehnlab.ucdavis.edu/documentation/license>

DIETHYL 2-METHYLPROPANEDIOATE

<https://mona.fiehnlab.ucdavis.edu/spectra/browse?>

[query=exists\(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27UPQZOUHVTJNGFK-UHFFFAOYSA-N%27\)](#)

14. NIST Mass Spectrometry Data Center**LICENSE**

Data covered by the Standard Reference Data Act of 1968 as amended.

<https://www.nist.gov/srd/public-law>

Propanedioic acid, methyl-, diethyl ester

<http://www.nist.gov/srd/nist1a.cfm>

15. SpectraBase

PROPANEDIOIC ACID, METHYL-, DIETHYL ESTER

<https://spectrabase.com/spectrum/AOqds5WrQ13>

PROPANEDIOIC ACID, METHYL-, DIETHYL ESTER

<https://spectrabase.com/spectrum/FrOhskL6v6s>

Diethyl methylmalonate

<https://spectrabase.com/spectrum/L8hHLeblIif>

Methy malonic acid, diethyl ester

<https://spectrabase.com/spectrum/I8DR2bFFxFg>

Diethyl methylmalonate

<https://spectrabase.com/spectrum/DcMgNMqIkqP>

Diethyl methylmalonate

<https://spectrabase.com/spectrum/EZZIPmD2Rrl>

METHYLMALONIC ACID, DIETHYL ESTER

<https://spectrabase.com/spectrum/LGZNw4nEYQ4>

Methyl-malonic acid, diethyl ester

<https://spectrabase.com/spectrum/8sxjQH0tOUU>

methylmalonic acid, diethyl ester

<https://spectrabase.com/spectrum/3ODieSDF55d>

2-Methyl-malonic acid diethyl ester

<https://spectrabase.com/spectrum/8pr0Lgo8QoY>

MALONIC ACID, METHYL-, DIETHYL ESTER

<https://spectrabase.com/spectrum/Eq0ptZ00SFu>

Diethyl methylmalonate

<https://spectrabase.com/spectrum/AYFghvSYnQL>

Propanedioic acid, methyl-, diethyl ester

<https://spectrabase.com/spectrum/2OKn9jq5m9S>

Propanedioic acid, methyl-, diethyl ester

<https://spectrabase.com/spectrum/53DJM13fGTo>

Diethyl methylmalonate

<https://spectrabase.com/spectrum/1k5UUIEJvuG>

16. Nature Synthesis

<https://pubchem.ncbi.nlm.nih.gov/substance/485187033>

17. NMRShiftDB

<https://pubchem.ncbi.nlm.nih.gov/substance/22390704>

18. Springer Nature

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=12043054-173010856>

19. SpringerMaterials

2-methyl-propanedioic acid diethyl ester

https://materials.springer.com/substanceprofile/docs/smsid_wwxdwznphkafvfkfg

20. Thieme Chemistry

LICENSE

The Thieme Chemistry contribution within PubChem is provided under a CC-BY-NC-ND 4.0 license, unless otherwise stated.

<https://creativecommons.org/licenses/by-nc-nd/4.0/>

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=12043054-173010856>

21. Wikidata

LICENSE

CCZero

<https://creativecommons.org/publicdomain/zero/1.0/>

Diethyl methylmalonate

<https://www.wikidata.org/wiki/Q63395288>

22. Wiley

<https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=141475>

23. PubChem

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

24. GHS Classification (UNECE)

GHS Classification Tree

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

25. NORMAN Suspect List Exchange

LICENSE

Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0

<https://creativecommons.org/licenses/by/4.0/>

NORMAN Suspect List Exchange Classification

<https://www.norman-network.com/nds/SLE/>

26. EPA Substance Registry Services

LICENSE

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

EPA SRS List Classification

https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

27. PATENTSCOPE (WIPO)

SID 403382707

<https://pubchem.ncbi.nlm.nih.gov/substance/403382707>