

Methylsulfonylmethane e c2h6o2s structure



**ASSIGN
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Contents

- Retention Index (Linear):

Molecular
Formula $C_2H_6O_2S$

Average mass 94.133 Da

Density $1.1 \pm 0.1 \text{ g/cm}^3$

Boiling Point $240.9 \pm 8.0 \text{ }^\circ\text{C}$ at
760 mmHg

Flash Point $143.3 \pm 0.0 \text{ }^\circ\text{C}$

Molar
Refractivity $20.1 \pm 0.4 \text{ cm}^3$

Polarizability $8.0 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$

Surface
Tension $31.0 \pm 3.0 \text{ dyne/cm}$

Molar Volume $82.6 \pm 3.0 \text{ cm}^3$

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Predicted – Mcule

- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

110 °C
TCIM1239,

M0509

108-111 °C
Alfa Aesar

108-110 °C
Oxford

University Chemical

Safety Data (No longer

updated)
More details

107-110 °C
Merck

Millipore
1505, 803284

109 °C
Jean-Claude

Bradley Open Melting

Point Dataset
15743,

21349

110 °C
Jean-Claude

Bradley Open Melting

Point Dataset
6920

108-111 °C
Alfa

Aesar
B21747

109

°CFooDBFDB006725

- **Experimental Boiling Point:**

238 °CAIfa Aesar

238 °COxford University

Chemical Safety Data

(No longer

updated)More details

238 °CAIfa AesarB21747

- **Experimental Flash Point:**

143 °CAIfa Aesar

143 °COxford University

Chemical Safety Data

(No longer

updated)More details

143 °CAIfa Aesar

143 °F (61. 6667 °C)Alfa

AesarB21747

- **Experimental Gravity:**

1. 45 g/mLAlfa

AesarB21747

- Predicted Physico-chemical Properties

- **Predicted Melting Point:**

107-109 °CJ&K

Scientific219442

110 °CTCI

110 °CTCIM1239, M0509

- Miscellaneous

- **Appearance:**

colourless

crystalsOxford

University Chemical

Safety Data (No longer
updated)More details

- **Stability:**

Stable. Combustible.

Incompatible with
strong oxidizing agents.

Oxford University

Chemical Safety Data

(No longer

updated)More details

- **Toxicity:**

ORL-RAT LD50 > 5000

mg kg⁻¹, SKN-RBT LD50

> 5000 mg kg⁻¹Oxford

University Chemical

Safety Data (No longer

updated)More details

- **Safety:**

CAUTION: May irritate

eyes, skin, and

respiratory tractAlfa

AesarB21747

Handle with caution.

Oxford University

Chemical Safety Data

(No longer

updated)More details

- **Therapeutical Effect:**

antiinflammatory,

antiproliferative,

antiparasiticMicrosource

[01505358]

- **Drug Status:**

agricultural

useMicrosource[01505358]

- **Compound Source:**

Cladonia deformis and

Equisetum

sppMicrosource[015053

58]

- Gas Chromatography

- **Retention Index (Kovats):**

727 (estimated with

error: 46)NIST

Spectramainlib_229649,

replib_19624,

replib_379569

1881. 4 (Program type:

Isothermal; Col... (show

more)umn class:

Standard polar; Column

length: 10 m; Column

type: Capillary; Start T:

130 C; CAS no: 67710;
Active phase: PEG-20M;
Phase thickness: 1.33
um; Data type: Kovats
RI; Authors: Huber, J. F.
K.; Kenndler, E.; Reich,
G.; Hack, W.; Wolf, J.,
Optimal Selection of Gas
Chromatographic
Columns for the
Analytical Control of
Chemical Warfare
Agents by Application of
Information Theory to
Retention Data, Anal.
Chem., 65(20), 1993,
2903-2906.)NIST
Spectranist ri
1900 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
length: 10 m; Column
type: Capillary; Start T:
160 C; CAS no: 67710;

Active phase: PEG-20M;
Phase thickness: 1.33
um; Data type: Kovats
RI; Authors: Huber, J. F.
K.; Kenndler, E.; Reich,
G.; Hack, W.; Wolf, J.,
Optimal Selection of Gas
Chromatographic
Columns for the
Analytical Control of
Chemical Warfare
Agents by Application of
Information Theory to
Retention Data, Anal.
Chem., 65(20), 1993,
2903-2906.)NIST
Spectranist ri

1913 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
length: 10 m; Column
type: Capillary; Start T:
180 C; CAS no: 67710;
Active phase: PEG-20M;

Phase thickness: 1.33
um; Data type: Kovats
RI; Authors: Huber, J. F.
K.; Kenndler, E.; Reich,
G.; Hack, W.; Wolf, J.,
Optimal Selection of Gas
Chromatographic
Columns for the
Analytical Control of
Chemical Warfare
Agents by Application of
Information Theory to
Retention Data, Anal.
Chem., 65(20), 1993,
2903-2906.)NIST
Spectranist ri

- **Retention Index (Normal Alkane):**

925 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0.25
mm; Column length: 30
m; Column type:
Capillary; CAS no:

67710; Active phase:
RTX-5 MS; Carrier gas:
Helium; Phase
thickness: 0.25 μm ;
Data type: Normal
alkane RI; Authors:
Mebazaa, R.; Mahmoudi,
A.; Fouchet, M.; Dos
Santos, M.; Kamissoko,
F.; Nafti, A.; Ben Cheikh,
R.; Rega, B.; Camel, V.,
Characterization of
volatile compounds in
Tunisian fenugreek
seeds, Food Chem.,
115, 2009, 1326-
1336.)NIST Spectranist
ri

931 (Program type:
Complex; Column...
(show more)class: Semi-
standard non-polar;
Column diameter: 0.25
mm; Column length: 30
m; Column type:

Capillary; Description:

50 0C (5 min) ^ 2

0C/min -> 100 0C (5

min) ^ 5 0C/min -> 300

0C; CAS no: 67710;

Active phase: RTX-5 MS;

Carrier gas: Helium;

Phase thickness: 0. 25

um; Data type: Normal

alkane RI; Authors:

Mebazaa, R.; Mahmoudi,

A.; Fouchet, M.; Dos

Santos, M.; Kamissoko,

F.; Nafti, A.; Ben Cheikh,

R.; Rega, B.; Camel, V.,

Characterization of

volatile compounds in

Tunisian fenugreek

seeds, Food Chem.,

115, 2009, 1326-

1336.)NIST Spectranist

ri

916 (Program type:

Ramp; Column cl...

(show more)ass: Semi-

standard non-polar;
Column diameter: 0.32
mm; Column length: 60
m; Column type:
Capillary; Heat rate: 3
K/min; Start T: 40 C;
End T: 230 C; End time:
10 min; Start time: 5
min; CAS no: 67710;
Active phase: SPB-5;
Phase thickness: 1.00
um; Data type: Normal
alkane RI; Authors:
Sivadier, G.; Ratel, J.;
Engel, E., Latency and
persistence of diet
volatile biomarkers in
lamb fats, J. Agric. Food
Chem., 57(2), 2009,
645-652.)NIST
Spectranist ri
909 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;

Column diameter: 0.32
mm; Column length: 60
m; Column type:
Capillary; CAS no:
67710; Active phase:
SPB-5; Phase thickness:
1 μm ; Data type:
Normal alkane RI;
Authors: Begnaud, F.;
Peres, C.; Berdague, J.-
L., Characterization of
volatile effluents of
livestock buildings by
solid-phase
microextraction, Int. J.
Environ. Anal. Chem.,
83(10), 2003, 837-
849.)NIST Spectranist ri
911 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0.32
mm; Column length: 60
m; Column type:

Capillary; Heat rate: 3
K/min; Start T: 30 C;
End T: 230 C; CAS no:
67710; Active phase:
SPB-5; Carrier gas:
Helium; Phase
thickness: 1.0 um; Data
type: Normal alkane RI;
Authors: Sebastian, I.;
Viallon-Fernandez, C.;
Berge, P.; Berdague, J.-
L., Analysis of the
volatile fraction of lamb
fat tissue: influence of
the type of feeding,
Sciences des Aliments,
23, 2003, 497-511.)NIST
Spectranist ri
918 (Program type:
Complex; Column...
(show more)class: Semi-
standard non-polar;
Column diameter: 0.25
mm; Column length: 30
m; Column type:

Capillary; Description:

50C=> 3C/min =>

160C => 6C/min =>

250C => 25C/min=>

325C; CAS no: 67710;

Active phase: DB-5MS;

Phase thickness: 1 um;

Data type: Normal

alkane RI; Authors:

Young, O. A.; Lane, G.

A.; Priolo, A.; Fraser, K.,

Pastoral and species

flavour in lambs raised

on pasture, lucerne or

maize, J. Sci. Food

Agric., 83, 2003, 93-

104.)NIST Spectranist ri

924 (Program type:

Ramp; Column cl...

(show more)ass: Semi-

standard non-polar;

Column diameter: 0. 32

mm; Column length: 30

m; Column type:

Capillary; Heat rate: 5

K/min; Start T: 40 C;
End T: 220 C; Start
time: 5 min; CAS no:
67710; Active phase:
DB-5; Carrier gas: H₂;
Phase thickness: 1 µm;
Data type: Normal
alkane RI; Authors:
Moio, L.; Langlois, D.;
Etievant, P.; Addeo, F.,
Powerful odorants in
bovine, ovine, caprine
and water buffalo milk
determined by means of
gas chromatography-
olfactometry, J. Dairy
Res., 60, 1993, 215-
222., Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0.32
mm; Column length: 50
m; Column type:
Capillary; Heat rate: 4
K/min; Start T: 40 C;

End T: 250 C; End time:
30 min; Start time: 3
min; CAS no: 67710;
Active phase: Ultra-2;
Carrier gas: He; Phase
thickness: 0.52 um;
Data type: Normal
alkane RI; Authors: King,
M.-F.; Matthews, M. A.;
Rule, D. C.; Field, R. A.,
Effect of beef packaging
method on volatile
compounds developed
by oven roasting or
microwave cooking, J.
Agric. Food Chem., 43,
1995, 773-778.)NIST
Spectranist ri
915 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0.32
mm; Column length: 50
m; Column type:

Capillary; Heat rate: 4
K/min; Start T: 40 C;
End T: 250 C; End time:
30 min; Start time: 3
min; CAS no: 67710;
Active phase: Ultra-2;
Carrier gas: He; Phase
thickness: 0.52 um;
Data type: Normal
alkane RI; Authors: King,
M.-F.; Hamilton, B. L.;
Matthews, M. A.; Rule,
D. C.; Field, R. A.,
Isolation and
identification of volatiles
and condensable
material in raw beef
with supercritical carbon
dioxide extraction, J.
Agric. Food Chem.,
41(11), 1993, 1974-
1981.)NIST Spectranist
ri

926 (Program type:
Ramp; Column cl...

(show more)ass: Semi-standard non-polar; Column diameter: 0.32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 220 C; CAS no: 67710; Active phase: DB-5; Carrier gas: H₂; Phase thickness: 1 μm; Data type: Normal alkane RI; Authors: Moio, L.; Dekimpe, J.; Etievant, P.; Addeo, F., Neutral volatile compounds in the raw milks from different species, J. Dairy Res., 60(2), 1993, 199-213.)NIST Spectranist ri 1887 (Program type: Complex; Column... (show more)class: Standard polar; Column

diameter: 0. 25 mm;
Column length: 30 m;
Column type: Capillary;
Description: 50 0C ^ 2
0C/min -> 100 0C (5
min) ^ 5 0C/min -> 250
0C; CAS no: 67710;
Active phase: DB-FFAP;
Carrier gas: Helium;
Phase thickness: 0. 25
um; Data type: Normal
alkane RI; Authors:
Mebazaa, R.; Mahmoudi,
A.; Fouchet, M.; Dos
Santos, M.; Kamissoko,
F.; Nafti, A.; Ben Cheikh,
R.; Rega, B.; Camel, V.,
Characterization of
volatile compounds in
Tunisian fenugreek
seeds, Food Chem.,
115, 2009, 1326-
1336.)NIST Spectranist
ri
1890 (Program type:

Ramp; Column cl...

(show more)ass:

Standard polar; Column

diameter: 0. 25 mm;

Column length: 30 m;

Column type: Capillary;

CAS no: 67710; Active

phase: DB-FFAP; Carrier

gas: Helium; Phase

thickness: 0. 25 um;

Data type: Normal

alkane RI; Authors:

Mebazaa, R.; Mahmoudi,

A.; Fouchet, M.; Dos

Santos, M.; Kamissoko,

F.; Nafti, A.; Ben Cheikh,

R.; Rega, B.; Camel, V.,

Characterization of

volatile compounds in

Tunisian fenugreek

seeds, Food Chem.,

115, 2009, 1326-

1336.)NIST Spectranist

ri

1911 (Program type:

Ramp; Column cl...

(show more)ass:

Standard polar; Column

diameter: 0. 32 mm;

Column length: 60 m;

Column type: Capillary;

Heat rate: 4 K/min; Start

T: 40 C; End T: 220 C;

End time: 20 min; Start

time: 8 min; CAS no:

67710; Active phase:

CP-Wax 52CB; Carrier

gas: He; Phase

thickness: 0. 5 um; Data

type: Normal alkane RI;

Authors: Povolo, M.;

Contarini, G.; Mele, M.;

Secchiari, P., Study on

the influence of pasture

on volatile fraction of

Ewes' dairy products by

solid-phase

microextraction and gas

chromatography-mass

spectrometry, J. Dairy

Sci., 90, 2007, 556-

569.)NIST Spectranist ri

1914 (Program type:

Ramp; Column cl...

(show more)ass:

Standard polar; Column

diameter: 0. 32 mm;

Column length: 60 m;

Column type: Capillary;

Heat rate: 4 K/min; Start

T: 40 C; End T: 220 C;

End time: 20 min; Start

time: 8 min; CAS no:

67710; Active phase:

CP-Wax 52CB; Carrier

gas: He; Phase

thickness: 0. 5 um; Data

type: Normal alkane RI;

Authors: Povolo, M.;

Contarini, G.; Mele, M.;

Secchiari, P., Study on

the influence of pasture

on volatile fraction of

Ewes' dairy products by

solid-phase

microextraction and gas

chromatography-mass
spectrometry, J. Dairy
Sci., 90, 2007, 556-
569.)NIST Spectranist ri
1895 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0. 25 mm;
Column length: 30 m;
Column type: Capillary;
Heat rate: 10 K/min;
Start T: 40 C; End T: 220
C; End time: 10 min;
Start time: 5 min; CAS
no: 67710; Active
phase: RTX-Wax; Carrier
gas: He; Phase
thickness: 0. 5 um; Data
type: Normal alkane RI;
Authors: Prosocki, R. A.;
Etzel, M. R.; Rankin, S.
A., Solvent type affects
the number,
distribution, and relative

quantities of volatile
compounds found in
sweet whey powder, J.

Dairy Sci., 90, 2007,
523-531.)NIST

Spectranist ri

1869. 2 (Program type:

Ramp; Column cl...

(show more)ass:

Standard polar; Column
diameter: 0. 03 in;

Column length: 1000 ft;

Column type: Capillary;

Heat rate: 4 K/min; Start

T: 80 C; End T: 225 C;

Start time: 5 min; CAS

no: 67710; Active

phase: Carbowax 20M;

Data type: Normal

alkane RI; Authors:

Mussinán, C. J.; Walradt,

J. P., Volatile

constituents of pressure

cooked pork liver, J.

Agric. Food Chem.,

22(5), 1974, 827-
831.)NIST Spectranist ri

- **Retention Index (Linear):**

919 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0. 25
mm; Column length: 30
m; Column type:
Capillary; Heat rate: 4
K/min; Start T: 40 C;
End T: 200 C; End time:
10 min; Start time: 1
min; CAS no: 67710;
Active phase: DB-5MS;
Carrier gas: He; Phase
thickness: 0. 25 um;
Data type: Linear RI;
Authors: Cho, I. H.;
Namgung, H.-J.; Choi,
H.-K.; Kim, Y.-S.,
Volatiles and key
odorants in the pileus
and stipe of pine-

mushroom (Tricholoma
matsutake Sing.), Food
Chem., 106, 2008, 71-
76.)NIST Spectranist ri
915 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0. 32
mm; Column length: 60
m; Column type:
Capillary; Heat rate: 3
K/min; Start T: 40 C;
End T: 230 C; End time:
10 min; Start time: 2
min; CAS no: 67710;
Active phase: SPB-5;
Phase thickness: 1 um;
Data type: Linear RI;
Authors: Engel, E.;
Ratel, J., Correction of
the data generated by
mass spectrometry
analyses of biological
tissues: Application to

food authentication, J.
Chromatogr. A, 1154,
2007, 331-341.)NIST
Spectranist ri

926 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0. 32
mm; Column length: 30
m; Column type:
Capillary; Heat rate: 3
K/min; Start T: 40 C;
End T: 210 C; CAS no:
67710; Active phase:
DB-5; Carrier gas: H2;
Phase thickness: 1 um;
Data type: Linear RI;
Authors: Moio, L.;
Piombino, P.; Addeo, F.,
Odour-impact
compounds of
Gorgonzola cheese, J.
Dairy Res., 67, 2000,
273-285., Program type:

Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0. 32
mm; Column length: 30
m; Column type:
Capillary; Heat rate: 3
K/min; Start T: 40 C;
End T: 220 C; CAS no:
67710; Active phase:
DB-5; Carrier gas: H2;
Phase thickness: 1 um;
Data type: Linear RI;
Authors: Moio L.; Rillo
L.; Ledda A.; Addeo F.,
Odorous constituents of
ovine milk in
relationship to diet, J.
Dairy Sci., 79, 1996,
1322-1331.)NIST
Spectranist ri
925 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;

Column diameter: 0.32
mm; Column length: 30
m; Column type:
Capillary; Heat rate: 4
K/min; Start T: 60 C;
End T: 250 C; End time:
20 min; Start time: 5
min; CAS no: 67710;
Active phase: DB-5;
Phase thickness: 1 um;
Data type: Linear RI;
Authors: Madruga, M. S.;
Mottram, D. S., The
effect of pH on the
formation of volatile
compounds produced by
heating a model system
containing 5'-imp and
cysteine, J. Braz. Chem.
Soc., 9(3), 1998, 261-
271.)NIST Spectranist ri
924 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;

Column diameter: 0.32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 220 C; CAS no: 67710; Active phase: DB-5; Carrier gas: H₂; Phase thickness: 1 μm; Data type: Linear RI; Authors: Moio L.; Rillo L.; Ledda A.; Addeo F., Odorous constituents of ovine milk in relationship to diet, J. Dairy Sci., 79, 1996, 1322-1331.)NIST Spectranist ri 921.6 (Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0.32 mm; Column length: 15 m; Column type:

Capillary; Heat rate: 10
K/min; Start T: 50 C;
End T: 300 C; Start
time: 2 min; CAS no:
67710; Active phase:
DB-5; Carrier gas: He;
Phase thickness: 0. 25
um; Data type: Linear
RI; Authors: D'Agostino,
P. A.; Provost, L. R., Gas
chromatographic
retention indices of
chemical warfare agents
and simulants, J.
Chromatogr., 331, 1985,
47-54.)NIST Spectranist
ri

1912 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0. 25 mm;
Column length: 30 m;
Column type: Capillary;
Heat rate: 4 K/min; Start

T: 40 C; End T: 200 C;
End time: 10 min; Start
time: 1 min; CAS no:
67710; Active phase:
DB-Wax; Carrier gas:
He; Phase thickness: 0.
25 um; Data type:
Linear RI; Authors: Cho,
I. H.; Namgung, H.-J.;
Choi, H.-K.; Kim, Y.-S.,
Volatiles and key
odorants in the pileus
and stipe of pine-
mushroom (*Tricholoma
matsutake* Sing.), Food
Chem., 106, 2008, 71-
76., Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0.25 mm;
Column length: 60 m;
Column type: Capillary;
Heat rate: 4 K/min; Start
T: 40 C; End T: 200 C;
End time: 10 min; Start

time: 1 min; CAS no:
67710; Active phase:
DB-Wax; Carrier gas:
He; Phase thickness: 0.
25 um; Data type:
Linear RI; Authors: Cho,
I. H.; Choi, H.-K.; Kim,
Y.-S., Difference in the
volatile composition of
pine-mushrooms
(Tricholoma matsutake
Sing.) according to their
grades, J. Agric. Food
Chem., 54, 2006, 4820-
4825.)NIST Spectranist
ri

1895 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0. 25 mm;
Column length: 30 m;
Column type: Capillary;
Heat rate: 4 K/min; Start
T: 40 C; End T: 250 C;

End time: 15 min; Start
time: 5 min; CAS no:
67710; Active phase:
DB-Wax; Carrier gas:
He; Phase thickness: 0.
5 um; Data type: Linear
RI; Authors: Pozo-Bayon
M. A.; Ruiz-Rodriguez A.;
Pernin K.; Cayot N.,
Influence of eggs on the
aroma composition of a
sponge cake and on the
aroma release in model
studies on flavored
sponge cakes, J. Agric.
Food Chem., 55, 2007,
1418-1426.)NIST
Spectranist ri
1908 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0. 25 mm;
Column length: 60 m;
Column type: Capillary;

Heat rate: 4 K/min; Start
T: 40 C; End T: 200 C;
End time: 10 min; Start
time: 1 min; CAS no:
67710; Active phase:
DB-Wax; Carrier gas:
He; Phase thickness: 0.
25 um; Data type:
Linear RI; Authors: Cho,
I. H.; Choi, H.-K.; Kim,
Y.-S., Difference in the
volatile composition of
pine-mushrooms
(Tricholoma matsutake
Sing.) according to their
grades, J. Agric. Food
Chem., 54, 2006, 4820-
4825.)NIST Spectranist
ri

1906 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0. 25 mm;
Column length: 60 m;

Column type: Capillary;
Heat rate: 2 K/min; Start
T: 35 C; End T: 195 C;
End time: 90 min; Start
time: 5 min; CAS no:
67710; Active phase:
Supelcowax-10; Carrier
gas: He; Phase
thickness: 0.25 um;
Data type: Linear RI;
Authors: Chung, H.-Y.;
Yung, I. K. S.; Ma, W. C.
J.; Kim, J.-S., Analysis of
volatile components in
frozen and dried
scallops (*Patinopecten
yessoensis*) by gas
chromatography/mass
spectrometry, Food Res.
Int., 35, 2002, 43-
53.)NIST Spectranist ri
1932 (Program type:
Complex; Column...
(show more)class:
Standard polar; Column

diameter: 0. 25 mm;
Column length: 50 m;
Column type: Capillary;
Description: 20C (5min)
=> 2C/min => 70C =>
4C/min => 210C; CAS
no: 67710; Active
phase: FFAP; Carrier
gas: He; Phase
thickness: 0. 25 um;
Data type: Linear RI;
Authors: Yasuhara, A.,
Identification of Volatile
Compounds in Poultry
Manure by Gas
Chromatography-Mass
Spectrometry, J.
Chromatogr., 387, 1987,
371-378.)NIST
Spectranist ri

Predicted data is generated using the ACD/Labs Percepta Platform -
PhysChem Module

Density: 1. 1±0. 1 g/cm³

Boiling Point: 240. 9±8. 0 °C at 760 mmHg

<https://assignbuster.com/methylsulfonylmethane-c2h6o2s-structure/>

Vapour Pressure:	0. 1±0. 5 mmHg at 25°C
Enthalpy of Vaporization:	45. 8±3. 0 kJ/mol
Flash Point:	143. 3±0. 0 °C
Index of Refraction:	1. 402
Molar Refractivity:	20. 1±0. 4 cm ³
#H bond acceptors:	2
#H bond donors:	0
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	-1. 19
ACD/LogD (pH 5. 5):	-0. 74
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	9. 43
ACD/LogD (pH 7. 4):	-0. 74
ACD/BCF (pH 7. 4):	1. 00

ACD/KOC (pH 7. 4):	9. 43
Polar Surface Area:	43 Å ²
Polarizability:	8. 0±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	31. 0±3. 0 dyne/cm
Molar Volume:	82. 6±3. 0 cm ³

Predicted data is generated using the US Environmental Protection Agency's

EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = -1. 11Log Kow (Exper. database match) = -1. 41Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 144. 57 (Adapted Stein & Brown method)Melting Pt (deg C): -20. 05 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00735 (Modified Grain method)MP (exp database): 109 deg CBP (exp database): 238 deg CSubcooled liquid VP: 0. 0491 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1e+006log Kow used: -1. 41 (expkow database)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 24E-006 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 9. 103E-010 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: -1. 41 (exp database)Log Kaw used: -3. 593 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 183Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7027Biowin2 (Non-Linear Model) : 0. 8419Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9912 (weeks)Biowin4 (Primary Survey Model) : 3. 7119 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4329Biowin6 (MITI Non-Linear Model): 0. 4619Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 6769Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 6. 55 Pa (0. 0491 mm Hg)Log Koa (Koawin est): 2. 183Kp (particle/gas partition coef. (m3/ug)): Mackay model : 4. 58E-007 Octanol/air (Koa) model: 3. 74E-011 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 66E-005 Mackay model : 3. 67E-005 Octanol/air (Koa) model: 2. 99E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 2. 1216 E-12 cm3/molecule-secHalf-Life = 5. 041 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 60. 498 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 66E-005 (Junge, Mackay)Note: the sorbed

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fraction may be resistant to atmospheric oxidation
Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 4. 926
Log Koc: 0. 693
Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Rate constants can NOT be estimated for this structure!
Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17):
Log BCF from regression-based method = 0. 500 (BCF = 3. 162)
log Kow used: -1. 41 (expkow database)
Volatilization from Water: Henry LC: 6. 24E-006 atm-m³/mole (estimated by Bond SAR Method)
Half-Life from Model River: 92. 02 hours (3. 834 days)
Half-Life from Model Lake : 1085 hours (45. 22 days)
Removal In Wastewater Treatment: Total removal: 2. 19 percent
Total biodegradation: 0. 09 percent
Total sludge adsorption: 1. 75 percent
Total to Air: 0. 35 percent (using 10000 hr Bio P, A, S)
Level III Fugacity Model: Mass Amount Half-Life Emissions (percent) (hr) (kg/hr)
Air 6. 54 121 1000 Water 45. 9 360 1000 Soil 47. 5 720 1000 Sediment 0. 084 3. 24e+003 0
Persistence Time: 354 hr

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- 1-Click Scaffold Hop