

S-Methyl methanethiosulfinate

Other names:	Dimethyldisulfide, S-oxide S-Methyl methanesulfinothioate Methyl methanethiosulfinate Methanesulfinothioic acid, S-methyl ester
Inchi:	InChI=1S/C2H6OS2/c1-4-5(2)3/h1-2H3
InchiKey:	RRGUMJYEQDVBFP-UHFFFAOYSA-N
Formula:	C2H6OS2
SMILES:	CSS(C)=O
Mol. weight [g/mol]:	110.20
CAS:	13882-12-7

Physical Properties

Property code	Value	Unit	Source
gf	-218.63	kJ/mol	Joback Method
hf	-248.48	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	39.59	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	0.643		Crippen Method
mcvol	77.610	ml/mol	McGowan Method
pc	5853.95	kPa	Joback Method
rinpol	934.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1339.00		NIST Webbook
tb	372.22	K	Joback Method
tc	578.36	K	Joback Method
tf	183.18	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.37	J/mol×K	372.22	Joback Method
cpg	126.59	J/mol×K	406.58	Joback Method
cpg	132.65	J/mol×K	440.93	Joback Method
cpg	138.55	J/mol×K	475.29	Joback Method
cpg	144.26	J/mol×K	509.64	Joback Method
cpg	149.77	J/mol×K	544.00	Joback Method
cpg	155.07	J/mol×K	578.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13882127&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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