S-METHYL METHANETHIOSULPHINATE

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

Physical Properties

Property code	Value	Unit	Source
hf	-166.96	kJ/mol	Cheméo Relay (1.0)
hfus	12.82	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
logp	0.643		Crippen Method
mcvol	77.610	ml/mol	McGowan Method
rinpol	934.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	940.00		NIST Webbook
ripol	1339.00		NIST Webbook
tb	441.49	K	Cheméo Relay (1.0)
tc	720.20	K	Cheméo Relay (1.0)
tf	247.61	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13882127&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point