S-Methyl methanethiosulphonate

Other names:	Methyl methanethiolsulfonate
	S-Methyl methanethiosulfonate
	Methanesulfonothioic acid, S-methyl ester
	Methanesulfonic acid, thio-, S-methyl ester
	Methyl methanesulfonothioate
	S-Methyl methanesulfonothioate
	Methyl methanethiosulfonate
	S-methyl methylthiosulfonate
	dimethyl thiosulfonate
Inchi:	InChI=1S/C2H6O2S2/c1-5-6(2,3)4/h1-2H3
InchiKey:	XYONNSVDNIRXKZ-UHFFFAOYSA-N
Formula:	C2H6O2S2
SMILES:	CSS(C)(=O)=O
Mol. weight [g/mol]:	126.20
CAS:	2949-92-0

Physical Properties

Property code	Value	Unit	Source
gf	-469.46	kJ/mol	Joback Method
hf	-496.09	kJ/mol	Joback Method
hfus	16.44	kJ/mol	Joback Method
hvap	45.50	kJ/mol	Joback Method
log10ws	-0.37		Crippen Method
logp	0.309		Crippen Method
mcvol	83.480	ml/mol	McGowan Method
pc	6524.67	kPa	Joback Method
rinpol	1068.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1065.50		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1065.50		NIST Webbook
rinpol	1081.00		NIST Webbook
tb	361.72	K	Joback Method
tc	552.01	K	Joback Method
tf	185.26	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.17	J/mol×K	361.72	Joback Method
cpg	139.64	J/mol×K	393.43	Joback Method
cpg	145.97	J/mol×K	425.15	Joback Method
cpg	152.14	J/mol×K	456.86	Joback Method
cpg	158.13	J/mol×K	488.58	Joback Method
cpg	163.94	J/mol×K	520.29	Joback Method
cpg	169.54	J/mol×K	552.01	Joback Method

Sources

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=C2949920&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume