Methane, (methylsulfinyl)(methylthio)-

Other names:	(Methylsulfanyl)(methylsulfinyl)methane
	(Methylsulfinyl)(methylthio)methane
	(Methylthio)dimethyl sulfoxide
	1-methylsulfinyl-2-thiapropane
	FAMSO
	Formaldehyde methyl mercaptal S-oxide
	NSC 181492
	Sulfide, methyl (methylsulfinyl)methyl
	formaldehyde dimethyl mercaptal S-oxide
	methyl (methylsulfinyl)methyl sulfide
	methyl (methylthio)methyl sulfoxide
	methyl methylthiomethyl sulphoxide
Inchi:	InChI=1S/C3H8OS2/c1-5-3-6(2)4/h3H2,1-2H3
InchiKey:	OTKFCIVOVKCFHR-UHFFFAOYSA-N
Formula:	C3H8OS2
SMILES:	CSCS(C)=O
Mol. weight [g/mol]:	124.22
CAS:	33577-16-1

Physical Properties

Property code	Value	Unit	Source
gf	-210.21	kJ/mol	Joback Method
hf	-269.12	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	41.81	kJ/mol	Joback Method
log10ws	-0.09		Crippen Method
logp	0.685		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	1182.80		NIST Webbook
tb	395.10	K	Joback Method
tc	599.58	K	Joback Method
tf	194.45	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.39	J/mol×K	395.10	Joback Method
cpg	161.38	J/mol×K	429.18	Joback Method
cpg	169.11	J/mol×K	463.26	Joback Method
cpg	176.58	J/mol×K	497.34	Joback Method
cpg	183.78	J/mol×K	531.42	Joback Method
cpg	190.68	J/mol×K	565.50	Joback Method
cpg	197.29	J/mol×K	599.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33577161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Excess Enthalpies of {CH3(CH2)nCN, n = 5 to 12} + Methyl Methylthiomethyl Sulfoxide or + Dimethyl Sulfoxide at 298.15 K:	https://www.doi.org/10.1021/je0499317
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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