Disulfide, methyl (methylthio)methyl

Other names:	Methyl methylthiomethyl disulfide
	2,4,5-Trithiahexane
	2,3,5-Trithiahexane
	Methane, (methyldithio)(methylthio)-
	Methyl (methylthio)methyl disulphide
	1-(methylthio)dimethyl disulfide
Inchi:	InChI=1S/C3H8S3/c1-4-3-6-5-2/h3H2,1-2H3
InchiKey:	MYIOBINSHMEDEY-UHFFFAOYSA-N
Formula:	C3H8S3
SMILES:	CSCSSC
Mol. weight [g/mol]:	140.29
CAS:	42474-44-2

Physical Properties

Property code	Value	Unit	Source
gf	73.74	kJ/mol	Joback Method
hf	20.36	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	42.72	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.318		Crippen Method
mcvol	102.180	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1130.00		NIST Webbook

rinpol	1147.00		NIST Webbook
rinpol	1134.10		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1134.10		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1099.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1705.50		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1705.50		NIST Webbook
ripol	1630.00		NIST Webbook
tb	474.38	K	Joback Method
tc	721.99	K	Joback Method
tf	226.77	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.54	J/mol×K	474.38	Joback Method
cpg	186.23	J/mol×K	515.65	Joback Method
cpg	194.55	J/mol×K	556.92	Joback Method
cpg	202.47	J/mol×K	598.18	Joback Method
cpg	209.97	J/mol×K	639.45	Joback Method
cpg	217.02	J/mol×K	680.72	Joback Method
cpg	223.61	J/mol×K	721.99	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42474442&Units=SI

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

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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume