Disulfide, methyl 2-methyl-1-(methylthio)propyl

Other names: 3-Isopropyl-2,4,5-trithiahexane
2,4,5-Trithiahexane, 3-(1-methylethyl), #1
Inchi: InChI=1S/C6H14S3/c1-5(2)6(7-3)9-8-4/h5-6H,1-4H3
InchiKey: XZMIKYIHVMVWFE-UHFFFAOYSA-N
Formula: C6H14S3
SMILES: CSSC(SC)C(C)C
Mol. weight [g/mol]: 182.37
CAS: 69078-81-5

Physical Properties

Property code	Value	Unit	Source
gf	94.12	kJ/mol	Joback Method
hf	-52.12	kJ/mol	Joback Method
hfus	16.64	kJ/mol	Joback Method
hvap	48.62	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.343		Crippen Method
mcvol	144.450	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
tb	542.14	K	Joback Method
tc	786.93	K	Joback Method
tf	230.58	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.13	J/mol×K	542.14	Joback Method
cpg	315.78	J/mol×K	582.94	Joback Method
cpg	328.66	J/mol×K	623.74	Joback Method
cpg	340.77	J/mol×K	664.54	Joback Method
cpg	352.09	J/mol×K	705.33	Joback Method

cpg	362.62	J/mol×K	746.13	Joback Method
cpg	372.35	J/mol×K	786.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69078815&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
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