Propane, 2,2-bis(methylthio)-

Other names:	Acetone, dimethyl mercaptole
	2,2-Bis(methylthio)propane
	2,2-Bis(methylsulfanyl)propane
	3,3-Dimethyl-2,4-dithiapentane
Inchi:	InChI=1S/C5H12S2/c1-5(2,6-3)7-4/h1-4H3
InchiKey:	BBYNYNMPOUQKKS-UHFFFAOYSA-N
Formula:	C5H12S2
SMILES:	CSC(C)(C)SC
Mol. weight [g/mol]:	136.28
CAS:	6156-18-9

Physical Properties

Property code	Value	Unit	Source
gf	60.30	kJ/mol	Joback Method
hf	-71.54	kJ/mol	Joback Method
hfus	9.55	kJ/mol	Joback Method
hvap	39.06	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.449		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
rinpol	986.00		NIST Webbook
tb	448.13	K	Joback Method
tc	678.67	K	Joback Method
tf	217.33	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.67	J/mol×K	448.13	Joback Method
cpg	228.91	J/mol×K	486.55	Joback Method
cpg	240.43	J/mol×K	524.98	Joback Method
cpg	251.25	J/mol×K	563.40	Joback Method

cpg	261.40	J/mol×K	601.82	Joback Method
cpg	270.88	J/mol×K	640.25	Joback Method
cpg	279.73	J/mol×K	678.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6156189&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

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