Bis(methylsulfonyl)methane

Inchi: InChI=1S/C3H8O4S2/c1-8(4,5)3-9(2,6)7/h3H2,1-2H3
InchiKey: VDPDRYUUTXEEIE-UHFFFAOYSA-N
Formula: C3H8O4S2
SMILES: CS(=O)(=O)CS(C)(=O)=O
Mol. weight [g/mol]: 172.22
CAS: 1750-62-5

Physical Properties

Property code	Value	Unit	Source
gf	-962.70	kJ/mol	Joback Method
hf	-1011.95	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	0.76		Crippen Method
logp	-0.967		Crippen Method
mcvol	109.310	ml/mol	McGowan Method
pc	6990.97	kPa	Joback Method
rinpol	1359.70		NIST Webbook
rinpol	1359.70		NIST Webbook
tb	363.60	K	Joback Method
tc	526.04	K	Joback Method
tf	200.69	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.11	J/mol×K	363.60	Joback Method
cpg	198.40	J/mol×K	390.67	Joback Method
cpg	206.51	J/mol×K	417.75	Joback Method
cpg	214.41	J/mol×K	444.82	Joback Method
cpg	222.11	J/mol×K	471.89	Joback Method
cpg	229.58	J/mol×K	498.96	Joback Method
cpg	236.82	J/mol×K	526.04	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=C1750625&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