bis-(1-Methyl-2-oxopropyl) disulfide, #1

Inchi: InChI=1S/C8H14O2S2/c1-5(9)7(3)11-12-8(4)6(2)10/h7-8H,1-4H3
InchiKey: NLXBKJGCEKRYJY-UHFFFAOYSA-N
Formula: C8H14O2S2
SMILES: CC(=O)C(C)SSC(C)C(C)=O
Mol. weight [g/mol]: 206.33

Physical Properties

Property code	Value	Unit	Source
gf	-180.00	kJ/mol	Joback Method
hf	-360.43	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	59.75	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.323		Crippen Method
mcvol	159.420	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
tb	626.86	K	Joback Method
tc	857.93	K	Joback Method
tf	318.58	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.78	J/mol×K	626.86	Joback Method
cpg	387.61	J/mol×K	665.37	Joback Method
cpg	399.60	J/mol×K	703.88	Joback Method
cpg	410.76	J/mol×K	742.40	Joback Method
cpg	421.10	J/mol×K	780.91	Joback Method
cpg	430.61	J/mol×K	819.42	Joback Method
cpg	439.30	J/mol×K	857.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R90662&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