bis(1-methyl-2-oxopropyl)trisulfide

Inchi: InChI=1S/C8H14O2S3/c1-5(9)7(3)11-13-12-8(4)6(2)10/h7-8H,1-4H3
InchiKey: WDCHVDPVOZRHQG-UHFFFAOYSA-N
Formula: C8H14O2S3
SMILES: CC(=O)C(C)SSSC(C)C(C)=O
Mol. weight [g/mol]: 238.39

Physical Properties

Property code	Value	Unit	Source
gf	-146.88	kJ/mol	Joback Method
hf	-318.56	kJ/mol	Joback Method
hfus	25.02	kJ/mol	Joback Method
hvap	66.57	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.971		Crippen Method
mcvol	175.770	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1731.00		NIST Webbook
tb	695.64	K	Joback Method
tc	943.23	K	Joback Method
tf	352.98	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.96	J/mol×K	695.64	Joback Method
cpg	435.47	J/mol×K	736.91	Joback Method
cpg	446.96	J/mol×K	778.17	Joback Method
cpg	457.42	J/mol×K	819.44	Joback Method
cpg	466.85	J/mol×K	860.70	Joback Method
cpg	475.24	J/mol×K	901.97	Joback Method
cpg	482.58	J/mol×K	943.23	Joback Method

Sources

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=R223135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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