bis(2-oxopropyl) disulfide

Inchi: InChI=1S/C6H10O2S2/c1-5(7)3-9-10-4-6(2)8/h3-4H2,1-2H3
InchiKey: BSMFRHHVHWASCC-UHFFFAOYSA-N
Formula: C6H10O2S2
SMILES: CC(=O)CSSCC(C)=O
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	-191.96	kJ/mol	Joback Method
hf	-308.59	kJ/mol	Joback Method
hfus	22.75	kJ/mol	Joback Method
hvap	56.08	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.546		Crippen Method
mcvol	131.240	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	1405.00		NIST Webbook
ripol	2347.00		NIST Webbook
ripol	2347.00		NIST Webbook
tb	581.98	K	Joback Method
tc	812.25	K	Joback Method
tf	326.04	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.02	J/mol×K	581.98	Joback Method
cpg	291.40	J/mol×K	620.36	Joback Method
cpg	301.15	J/mol×K	658.74	Joback Method
cpg	310.29	J/mol×K	697.11	Joback Method
cpg	318.80	J/mol×K	735.49	Joback Method
cpg	326.68	J/mol×K	773.87	Joback Method
cpg	333.92	J/mol×K	812.25	Joback Method

Sources

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=R224143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume