bis-(2-Oxobutyl) disulfide

Inchi: InChI=1S/C8H14O2S2/c1-3-7(9)5-11-12-6-8(10)4-2/h3-6H2,1-2H3
InchiKey: CHRHQBLBXBGDHK-UHFFFAOYSA-N
Formula: C8H14O2S2
SMILES: CCC(=O)CSSCC(=O)CC
Mol. weight [g/mol]: 206.33

Physical Properties

Property code	Value	Unit	Source
gf	-175.12	kJ/mol	Joback Method
hf	-349.87	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	60.53	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.326		Crippen Method
mcvol	159.420	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	627.74	K	Joback Method
tc	849.42	K	Joback Method
tf	348.58	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.79	J/mol×K	627.74	Joback Method
cpg	386.00	J/mol×K	664.69	Joback Method
cpg	397.47	J/mol×K	701.63	Joback Method
cpg	408.20	J/mol×K	738.58	Joback Method
cpg	418.20	J/mol×K	775.53	Joback Method
cpg	427.46	J/mol×K	812.47	Joback Method
cpg	435.99	J/mol×K	849.42	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=R90694&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