2-Cyclohexen-1-one, 2-methyl-5-[1-methyl-1,2-bis-(methylthio)ethyl]

Inchi: InChI=1S/C12H20OS2/c1-9-5-6-10(7-11(9)13)12(2,15-4)8-14-3/h5,10H,6-8H2,1-4H3
InchiKey: NIJLSQHJXDHVEC-UHFFFAOYSA-N
Formula: C12H20OS2
SMILES: CSCC(C)(SC)C1CC=C(C)C(=O)C1
Mol. weight [g/mol]: 244.42

Physical Properties

Property code	Value	Unit	Source
gf	41.43	kJ/mol	Joback Method
hf	-253.09	kJ/mol	Joback Method
hfus	19.86	kJ/mol	Joback Method
hvap	60.27	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.396		Crippen Method
mcvol	199.050	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
tb	699.80	K	Joback Method
tc	957.84	K	Joback Method
tf	385.10	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.51	J/mol×K	699.80	Joback Method
cpg	560.67	J/mol×K	742.81	Joback Method
cpg	578.26	J/mol×K	785.81	Joback Method
cpg	594.29	J/mol×K	828.82	Joback Method
cpg	608.79	J/mol×K	871.82	Joback Method
cpg	621.74	J/mol×K	914.83	Joback Method
cpg	633.18	J/mol×K	957.84	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=R121623&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume