l-Cysteine, N,S-bis(pivaloyl)-, methyl ester

Inchi: InChI=1S/C14H25NO4S/c1-13(2,3)11(17)15-9(10(16)19-7)8-20-12(18)14(4,5)6/h9H,8H2
InchiKey: HZRYTLGAZBMHFD-UHFFFAOYSA-N
Formula: C14H25NO4S
SMILES: COC(=O)C(CSC(=O)C(C)(C)C)NC(=O)C(C)(C)C
Mol. weight [g/mol]: 303.42

Physical Properties

Property code	Value	Unit	Source
gf	-299.01	kJ/mol	Joback Method
hf	-729.69	kJ/mol	Joback Method
hfus	28.88	kJ/mol	Joback Method
hvap	79.68	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.996		Crippen Method
mcvol	245.030	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	1832.00		NIST Webbook
rinpol	1832.00		NIST Webbook
tb	815.80	K	Joback Method
tc	1032.31	K	Joback Method
tf	496.46	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.50	J/mol×K	815.80	Joback Method
cpg	747.47	J/mol×K	851.88	Joback Method
cpg	760.37	J/mol×K	887.97	Joback Method
cpg	772.23	J/mol×K	924.05	Joback Method
cpg	783.13	J/mol×K	960.14	Joback Method
cpg	793.12	J/mol×K	996.22	Joback Method
cpg	802.24	J/mol×K	1032.31	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=U299749&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume