l-Serine, N,O-bis(pivaloyl)-, methyl ester

Inchi: InChI=1S/C14H25NO5/c1-13(2,3)11(17)15-9(10(16)19-7)8-20-12(18)14(4,5)6/h9H,8H2,1
InchiKey: MCIIKIHFRAEYIB-UHFFFAOYSA-N
Formula: C14H25NO5
SMILES: COC(=O)C(COC(=O)C(C)(C)C)NC(=O)C(C)(C)C
Mol. weight [g/mol]: 287.35

Physical Properties

Property code	Value	Unit	Source
gf	-437.13	kJ/mol	Joback Method
hf	-903.78	kJ/mol	Joback Method
hfus	25.94	kJ/mol	Joback Method
hvap	75.27	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.280		Crippen Method
mcvol	234.550	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
tb	769.44	K	Joback Method
tc	971.71	K	Joback Method
tf	484.29	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.98	J/mol×K	769.44	Joback Method
cpg	719.56	J/mol×K	803.15	Joback Method
cpg	733.14	J/mol×K	836.86	Joback Method
cpg	745.76	J/mol×K	870.57	Joback Method
cpg	757.46	J/mol×K	904.29	Joback Method
cpg	768.28	J/mol×K	938.00	Joback Method
cpg	778.26	J/mol×K	971.71	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=U299746&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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