Propanoic acid, 2-amino-3-hydroxy, isopropyl ester

Inchi: InChI=1S/C6H13NO3/c1-4(2)10-6(9)5(7)3-8/h4-5,8H,3,7H2,1-2H3
InchiKey: DETDCGYOOXTNBW-UHFFFAOYSA-N
Formula: C6H13NO3
SMILES: CC(C)OC(=O)C(N)CO
Mol. weight [g/mol]: 147.17

Physical Properties

Property code	Value	Unit	Source
gf	-309.53	kJ/mol	Joback Method
hf	-540.97	kJ/mol	Joback Method
hfus	16.32	kJ/mol	Joback Method
hvap	64.65	kJ/mol	Joback Method
log10ws	-0.12		Crippen Method
logp	-0.742		Crippen Method
mcvol	118.690	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1147.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1150.00		NIST Webbook
tb	576.80	K	Joback Method
tc	764.37	K	Joback Method
tf	343.62	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.11	J/mol×K	576.80	Joback Method
cpg	307.73	J/mol×K	608.06	Joback Method
cpg	316.90	J/mol×K	639.32	Joback Method
cpg	325.64	J/mol×K	670.59	Joback Method
cpg	333.95	J/mol×K	701.85	Joback Method
cpg	341.83	J/mol×K	733.11	Joback Method

cpg	349.29	J/mol×K	764.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R535889&Units=SI
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

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