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

Inchi: InChI=1S/C7H15NO3/c1-4(2)11-7(10)6(8)5(3)9/h4-6,9H,8H2,1-3H3
InchiKey: DAVNUZXTMACPML-UHFFFAOYSA-N
Formula: C7H15NO3
SMILES: CC(C)OC(=O)C(N)C(C)O
Mol. weight [g/mol]: 161.20

Physical Properties

Property code	Value	Unit	Source
gf	-303.55	kJ/mol	Joback Method
hf	-566.89	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	66.49	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	-0.354		Crippen Method
mcvol	132.780	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1126.00		NIST Webbook
tb	599.24	K	Joback Method
tc	788.21	K	Joback Method
tf	339.89	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.71	J/mol×K	599.24	Joback Method
cpg	355.43	J/mol×K	630.73	Joback Method
cpg	365.64	J/mol×K	662.23	Joback Method
cpg	375.34	J/mol×K	693.72	Joback Method
cpg	384.54	J/mol×K	725.22	Joback Method
cpg	393.24	J/mol×K	756.71	Joback Method

cpg	401.44	J/mol×K	788.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R535809&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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