Alpha-i-butyl-alpha-methylglycine

Other names: DL-«alpha»-methylleucine
Inchi: InChI=1S/C7H15NO2/c1-5(2)4-7(3,8)6(9)10/h5H,4,8H2,1-3H3,(H,9,10)
InchiKey: ARSWQPLPYROOBG-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: CC(C)CC(C)(N)C(=O)O
Mol. weight [g/mol]: 145.20
CAS: 144-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-190.83	kJ/mol	Joback Method
hf	-432.86	kJ/mol	Joback Method
hfus	13.83	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	0.835		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	574.47	K	Joback Method
tc	767.73	K	Joback Method
tf	350.08	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.10	J/mol×K	574.47	Joback Method
cpg	334.97	J/mol×K	606.68	Joback Method
cpg	345.21	J/mol×K	638.89	Joback Method
cpg	354.85	J/mol×K	671.10	Joback Method
cpg	363.92	J/mol×K	703.31	Joback Method
cpg	372.45	J/mol×K	735.52	Joback Method
cpg	380.47	J/mol×K	767.73	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=C144241&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