boc-glycine

Inchi: InChI=1S/C7H13NO4/c1-7(2,3)12-6(11)8-4-5(9)10/h4H2,1-3H3,(H,8,11)(H,9,10)
InchiKey: VRPJIFMKZZEXLR-UHFFFAOYSA-N
Formula: C7H13NO4
SMILES: CC(C)(C)OC(=O)NCC(=O)O
Mol. weight [g/mol]: 175.18

Physical Properties

Property code	Value	Unit	Source
gf	-399.37	kJ/mol	Joback Method
hf	-652.70	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-0.08		Aqueous Solubility Prediction Method
logp	0.596		Crippen Method
mcvol	134.350	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	628.84	K	Joback Method
tc	817.53	K	Joback Method
tf	361.48	K	Aqueous Solubility Prediction Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.47	J/mol×K	628.84	Joback Method
cpg	361.14	J/mol×K	660.29	Joback Method
cpg	370.26	J/mol×K	691.74	Joback Method
cpg	378.84	J/mol×K	723.19	Joback Method
cpg	386.91	J/mol×K	754.63	Joback Method
cpg	394.48	J/mol×K	786.08	Joback Method
cpg	401.56	J/mol×K	817.53	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume