L-(-)-n-benzoyl-alpha-alanine

Inchi: InChI=1S/C10H11NO3/c1-7(10(13)14)11-9(12)8-5-3-2-4-6-8/h2-7H,1H3,(H,11,12)(H,13,1
InchiKey: UAQVHNZEONHPQG-ZETCQYMHSA-N
Formula: C10H11NO3
SMILES: CC(NC(=O)c1ccccc1)C(=O)O
Mol. weight [g/mol]: 193.20

Physical Properties

Property code	Value	Unit	Source
gf	-161.98	kJ/mol	Joback Method
hf	-342.40	kJ/mol	Joback Method
hfus	24.56	kJ/mol	Joback Method
hvap	76.35	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	0.889		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
tb	704.53	K	Joback Method
tc	915.36	K	Joback Method
tf	427.22	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.05	J/mol×K	704.53	Joback Method
cpg	397.07	J/mol×K	739.67	Joback Method
cpg	406.36	J/mol×K	774.81	Joback Method
cpg	414.95	J/mol×K	809.95	Joback Method
cpg	422.88	J/mol×K	845.08	Joback Method
cpg	430.19	J/mol×K	880.22	Joback Method
cpg	436.90	J/mol×K	915.36	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=B6002614&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