2-acetamido-3-(4-hydroxyphenyl)propanoic acid

Inchi: InChI=1S/C11H13NO4/c1-7(13)12-10(11(15)16)6-8-2-4-9(14)5-3-8/h2-5,10,14H,6H2,1H3

InchiKey: CAHKINHBCWCHCF-UHFFFAOYSA-N

Formula: C11H13NO4

SMILES: CC(=O)NC(Cc1ccc(O)cc1)C(=O)O

Mol. weight [g/mol]: 223.23

Physical Properties

Property code	Value	Unit	Source
gf	-308.18	kJ/mol	Joback Method
hf	-540.35	kJ/mol	Joback Method
hfus	32.93	kJ/mol	Joback Method
hvap	91.59	kJ/mol	Joback Method
log10ws	9.00e-03		Aqueous Solubility Prediction Method
logp	0.524		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	808.03	K	Joback Method
tc	1024.71	K	Joback Method
tf	550.21	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.95	J/mol×K	808.03	Joback Method
cpg	489.33	J/mol×K	844.14	Joback Method
cpg	498.18	J/mol×K	880.26	Joback Method
cpg	506.60	J/mol×K	916.37	Joback Method
cpg	514.66	J/mol×K	952.48	Joback Method
cpg	522.45	J/mol×K	988.59	Joback Method
cpg	530.03	J/mol×K	1024.71	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