3-(Dimethylaminomethyl)-4-hydroxy acetanilide

Inchi: InChI=1S/C11H16N2O2/c1-8(14)12-10-4-5-11(15)9(6-10)7-13(2)3/h4-6,15H,7H2,1-3H3,(

InchiKey: IUVBAHXLBOTWMB-UHFFFAOYSA-N

Formula: C11H16N2O2

SMILES: CC(=O)Nc1ccc(O)c(CN(C)C)c1

Mol. weight [g/mol]: 208.26

CAS: 13886-04-9

Physical Properties

Property code	Value	Unit	Source
gf	61.15	kJ/mol	Joback Method
hf	-214.20	kJ/mol	Joback Method
hfus	33.40	kJ/mol	Joback Method
hvap	71.26	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	1.412		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
tb	679.84	K	Joback Method
tc	898.56	K	Joback Method
tf	499.45	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.37	J/mol×K	679.84	Joback Method
cpg	472.33	J/mol×K	716.29	Joback Method
cpg	484.46	J/mol×K	752.75	Joback Method
cpg	495.86	J/mol×K	789.20	Joback Method
cpg	506.61	J/mol×K	825.66	Joback Method
cpg	516.78	J/mol×K	862.11	Joback Method
cpg	526.48	J/mol×K	898.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13886049&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume