5-Acetylamino-salicylic acid

Other names: 5-acetamidosalicylic acid
Inchi: InChI=1S/C9H9NO4/c1-5(11)10-6-2-3-8(12)7(4-6)9(13)14/h2-4,12H,1H3,(H,10,11)(H,13,
InchiKey: GEFDRROBUCULOD-UHFFFAOYSA-N
Formula: C9H9NO4
SMILES: CC(=O)Nc1ccc(O)c(C(=O)O)c1
Mol. weight [g/mol]: 195.17
CAS: 51-59-2

Physical Properties

Property code	Value	Unit	Source
gf	-332.21	kJ/mol	Joback Method
hf	-505.26	kJ/mol	Joback Method
hfus	30.89	kJ/mol	Joback Method
hvap	88.19	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.049		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
pc	5205.63	kPa	Joback Method
tb	767.69	K	Joback Method
tc	986.90	K	Joback Method
tf	555.19	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.22	J/mol×K	767.69	Joback Method
cpg	382.06	J/mol×K	804.23	Joback Method
cpg	389.45	J/mol×K	840.76	Joback Method
cpg	396.47	J/mol×K	877.30	Joback Method
cpg	403.16	J/mol×K	913.83	Joback Method
cpg	409.61	J/mol×K	950.37	Joback Method
cpg	415.88	J/mol×K	986.90	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=C51592&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