2-Acetamido-6-chlorobenzoic acid

Other names: Benzoic acid, 2-(acetylamino)-6-chloro-
Inchi: InChI=1S/C9H8ClNO3/c1-5(12)11-7-4-2-3-6(10)8(7)9(13)14/h2-4H,1H3,(H,11,12)(H,13,1
InchiKey: VFHSJTHAMJFUCK-UHFFFAOYSA-N
Formula: C9H8ClNO3
SMILES: CC(=O)Nc1cccc(Cl)c1C(=O)O
Mol. weight [g/mol]: 213.62
CAS: 19407-42-2

Physical Properties

Property code	Value	Unit	Source
gf	-199.15	kJ/mol	Joback Method
hf	-355.16	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	80.22	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.997		Crippen Method
mcvol	145.140	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	729.48	K	Joback Method
tc	944.47	K	Joback Method
tf	485.91	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.75	J/mol×K	729.48	Joback Method
cpg	361.83	J/mol×K	765.31	Joback Method
cpg	369.31	J/mol×K	801.14	Joback Method
cpg	376.21	J/mol×K	836.98	Joback Method
cpg	382.55	J/mol×K	872.81	Joback Method
cpg	388.36	J/mol×K	908.64	Joback Method
cpg	393.66	J/mol×K	944.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19407422&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