2-Amino-6-chlorobenzoic acid

Other names: Benzoic acid, 2-amino-6-chloro-
Inchi: InChI=1S/C7H6ClNO2/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,9H2,(H,10,11)
InchiKey: SZCPTRGBOVXVCA-UHFFFAOYSA-N
Formula: C7H6ClNO2
SMILES: Nc1cccc(Cl)c1C(=O)O
Mol. weight [g/mol]: 171.58
CAS: 2148-56-3

Physical Properties

Property code	Value	Unit	Source
gf	-110.01	kJ/mol	Joback Method
hf	-220.98	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.620		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
tb	652.21	K	Joback Method
tc	875.53	K	Joback Method
tf	444.04	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.90	J/mol×K	652.21	Joback Method
cpg	265.20	J/mol×K	689.43	Joback Method
cpg	271.97	J/mol×K	726.65	Joback Method
cpg	278.24	J/mol×K	763.87	Joback Method
cpg	284.04	J/mol×K	801.09	Joback Method
cpg	289.38	J/mol×K	838.31	Joback Method
cpg	294.28	J/mol×K	875.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2148563&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