2-Amino-4-chlorobenzoic acid

Other names:	4-Chloro anthranilic acid
	4-chloroanthranil acid
	4-chloroanthranilic acid
	Anthranilic acid, 4-chloro-
	Benzoic acid, 2-amino-4-chloro-
Inchi:	InChI=1S/C7H6ClNO2/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3H,9H2,(H,10,11)
InchiKey:	JYYLQSCZISREGY-UHFFFAOYSA-N
Formula:	C7H6ClNO2
SMILES:	Nc1cc(Cl)ccc1C(=O)O
Mol. weight [g/mol]:	171.58
CAS:	89-77-0

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	507.50	K	Solubility determination and thermodynamic modelling for 2-amino-4-chlorobenzoic acid in eleven organic solvents from T = (278.15 to 313.15) K and mixing properties of solutions
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

Solubility Measurement and Modeling of 2-Amino-4,6-dichoropyrimidine in Ten Pure Solvents and (Ethyl Acetate + Ethanol) Solvent Mixtures:	https://www.doi.org/10.1021/acs.jced.8b00292
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=C89770&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility determination and thermodynamic modelling for 2-amino-4-chlorobenzoic acid in eleven organic solvents from T = (278.15 to 313.15) K and mixing properties of solutions:	https://www.doi.org/10.1016/j.jct.2016.11.019

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

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