2-Chloro-5-nitrobenzoic acid

Other names:	6-Chloro-3-nitrobenzoic acid
	Benzoic acid, 2-chloro-5-nitro-
Inchi:	InChI=1S/C7H4ClNO4/c8-6-2-1-4(9(12)13)3-5(6)7(10)11/h1-3H,(H,10,11)
InchiKey:	QUEKGYQTRJVEQC-UHFFFAOYSA-N
Formula:	C7H4ClNO4
SMILES:	O=C(O)c1cc([N+](=O)[O-])ccc1Cl
Mol. weight [g/mol]:	201.56
CAS:	2516-96-3

Physical Properties

Property code	Value	Unit	Source
gf	-140.91	kJ/mol	Joback Method
hf	-265.53	kJ/mol	Joback Method
hfus	28.39	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-1.75		Aqueous Solubility Prediction Method
logp	1.946		Crippen Method
mcvol	122.830	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
tb	731.52	K	Joback Method
tc	968.96	K	Joback Method
tf	439.65	K	Aqueous Solubility Prediction Method
tf	440.10	K	Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	283.94	J/mol×K	731.52	Joback Method
cpg	290.51	J/mol×K	771.09	Joback Method
cpg	296.51	J/mol×K	810.67	Joback Method
cpg	301.95	J/mol×K	850.24	Joback Method
cpg	306.87	J/mol×K	889.81	Joback Method
cpg	311.30	J/mol×K	929.39	Joback Method
cpg	315.25	J/mol×K	968.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2516963&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