Benzoic acid, 4-chloro-

Other names:	4-Chlorobenzoic acid
	Acido p-clorobenzoico
	Benzoic acid, p-chloro-
	Chlorodracylic acid
	p-Carboxychlorobenzene
	p-Chlorbenzoic acid
	p-Chlorobenzoic acid
Inchi:	InChI=1S/C7H5ClO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
InchiKey:	XRHGYUZYPHTUJZ-UHFFFAOYSA-N
Formula:	C7H5ClO2
SMILES:	O=C(O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	156.57
CAS:	74-11-3

Physical Properties

Property code	Value	Unit	Source
gf	-166.83	kJ/mol	Joback Method
hf	-324.80 ± 0.80	kJ/mol	NIST Webbook
hfs	-427.30 ± 0.20	kJ/mol	NIST Webbook
hfs	-427.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-430.00 ± 1.00	kJ/mol	NIST Webbook
hfs	-430.00 ± 1.80	kJ/mol	NIST Webbook
hfs	-430.70 ± 1.20	kJ/mol	NIST Webbook
hfs	-428.90 ± 1.00	kJ/mol	NIST Webbook
hfs	-429.30 ± 1.60	kJ/mol	NIST Webbook
hfs	-427.90 ± 0.80	kJ/mol	NIST Webbook
hfus	30.91	kJ/mol	Thermodynamic study of the sublimation of six halobenzoic acids
hsub	105.20 ± 0.70	kJ/mol	NIST Webbook
hsub	107.90	kJ/mol	NIST Webbook
hsub	102.50 ± 0.40	kJ/mol	NIST Webbook
hsub	102.50 ± 0.40	kJ/mol	NIST Webbook
hvap	61.92	kJ/mol	Joback Method
log10ws	-3.42		Aqueous Solubility Prediction Method
logp	2.038		Crippen Method
mcvol	105.410	ml/mol	McGowan Method

pc	4717.12	kPa	Joback Method
rinpol	1336.00		NIST Webbook
rinpol	1336.00		NIST Webbook
tb	574.70	K	Joback Method
tc	789.74	K	Joback Method
tf	514.90	K	Aqueous Solubility Prediction Method
tf	512.85	K	KDB
tf	512.50	K	Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements
tf	511.00 ± 3.00	K	NIST Webbook
tf	512.00 ± 3.00	K	NIST Webbook
tf	512.90 ± 4.00	K	NIST Webbook
tf	512.85 ± 0.40	K	NIST Webbook
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.81	J/mol×K	682.22	Joback Method
cpg	221.19	J/mol×K	610.54	Joback Method
cpg	213.61	J/mol×K	574.70	Joback Method
cpg	240.90	J/mol×K	718.06	Joback Method
cpg	246.53	J/mol×K	753.90	Joback Method
cpg	251.74	J/mol×K	789.74	Joback Method
cpg	228.25	J/mol×K	646.38	Joback Method
cps	167.80	J/mol×K	298.00	NIST Webbook
dvisc	0.0017443	Pa×s	386.00	Joback Method
dvisc	0.0008553	Pa×s	423.74	Joback Method
dvisc	0.0004712	Pa×s	461.48	Joback Method
dvisc	0.0002841	Pa×s	499.22	Joback Method
dvisc	0.0001839	Pa×s	536.96	Joback Method
dvisc	0.0041518	Pa×s	348.26	Joback Method
dvisc	0.0001260	Pa×s	574.70	Joback Method
hfust	32.26	kJ/mol	512.90	NIST Webbook
hfust	32.26	kJ/mol	512.90	NIST Webbook
hfust	13.50	kJ/mol	330.00	NIST Webbook
hfust	30.91	kJ/mol	512.50	NIST Webbook

hfust	32.26	kJ/mol	512.90	NIST Webbook
hfust	34.26	kJ/mol	513.50	NIST Webbook
hfust	34.26	kJ/mol	513.53	NIST Webbook
hsubt	88.00 ± 2.00	kJ/mol	333.00	NIST Webbook
hsubt	101.90	kJ/mol	413.00	NIST Webbook
hsubt	103.30 ± 0.50	kJ/mol	344.50	NIST Webbook
sfust	62.90	J/mol×K	512.90	NIST Webbook

Sources

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=C74113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic study of the sublimation of six halobenzoic acids:	https://www.doi.org/10.1016/j.jct.2004.09.005
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1804

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume