Benzoic acid, 3-chloro-

Other names:	3-Chlorobenzoic acid
	Acido m-clorobenzoico
	Benzoic acid, m-chloro-
	m-Chlorobenzoic acid
Inchi:	InChI=1S/C7H5ClO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)
InchiKey:	LULAYUGMBFYYEX-UHFFFAOYSA-N
Formula:	C7H5ClO2
SMILES:	O=C(O)c1cccc(Cl)c1
Mol. weight [g/mol]:	156.57
CAS:	535-80-8

Physical Properties

Property code	Value	Unit	Source
chs	-3009.65 ± 0.57	kJ/mol	NIST Webbook
chs	-3068.10 ± 1.50	kJ/mol	NIST Webbook
chs	-3069.40 ± 8.40	kJ/mol	NIST Webbook
gf	-166.83	kJ/mol	Joback Method
hf	-321.80 ± 0.90	kJ/mol	NIST Webbook
hfs	-423.20 ± 0.80	kJ/mol	NIST Webbook
hfs	-424.60 ± 1.60	kJ/mol	NIST Webbook
hfus	23.67	kJ/mol	Thermodynamic study of the sublimation of six halobenzoic acids
hsub	101.40 ± 0.40	kJ/mol	NIST Webbook
hsub	105.80	kJ/mol	NIST Webbook
hsub	101.40 ± 0.40	kJ/mol	NIST Webbook
hsub	102.50 ± 0.50	kJ/mol	NIST Webbook
hvap	61.92	kJ/mol	Joback Method
log10ws	-2.62		Aqueous Solubility Prediction Method
logp	2.038		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	574.70	K	Joback Method
tc	789.74	K	Joback Method
tf	427.40	K	KDB
tf	427.40 ± 0.30	K	NIST Webbook
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.90	J/mol×K	718.06	Joback Method
cpg	228.25	J/mol×K	646.38	Joback Method
cpg	221.19	J/mol×K	610.54	Joback Method
cpg	213.61	J/mol×K	574.70	Joback Method
cpg	246.53	J/mol×K	753.90	Joback Method
cpg	251.74	J/mol×K	789.74	Joback Method
cpg	234.81	J/mol×K	682.22	Joback Method
cps	163.60	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	23.85	kJ/mol	427.40	NIST Webbook
hfust	23.85	kJ/mol	427.40	NIST Webbook
hfust	23.67	kJ/mol	427.90	NIST Webbook
hfust	22.00	kJ/mol	427.83	NIST Webbook
hfust	23.85	kJ/mol	427.40	NIST Webbook
hfust	22.00	kJ/mol	427.80	NIST Webbook
hsubt	81.00 ± 2.00	kJ/mol	328.00	NIST Webbook
hsubt	99.60	kJ/mol	413.00	NIST Webbook
hsubt	101.20 ± 0.40	kJ/mol	330.00	NIST Webbook
sfust	55.80	J/mol×K	427.40	NIST Webbook

Sources

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1805

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume