Benzoic acid, 2-chloro-

Other names:	2-CBA
	2-Chlorobenzoic acid
	Benzoic acid, o-chloro-
	Chlorobenzoic acid
	Kyselina o-chlorbenzoova
	o-Chlorobenzoic acid
Inchi:	InChI=1S/C7H5ClO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H,9,10)
InchiKey:	IKCLCGXPQILATA-UHFFFAOYSA-N
Formula:	C7H5ClO2
SMILES:	O=C(O)c1ccccc1Cl
Mol. weight [g/mol]:	156.57
CAS:	118-91-2

Physical Properties

Property code	Value	Unit	Source
chs	-3087.91 ± 0.69	kJ/mol	NIST Webbook
chs	-3087.76 ± 0.25	kJ/mol	NIST Webbook
chs	-3094.10 ± 8.40	kJ/mol	NIST Webbook
chs	-3073.10 ± 4.60	kJ/mol	NIST Webbook
gf	-166.83	kJ/mol	Joback Method
hf	-304.20 ± 0.70	kJ/mol	NIST Webbook
hfs	-405.10 ± 0.50	kJ/mol	NIST Webbook
hfs	-404.83 ± 0.74	kJ/mol	NIST Webbook
hfus	25.25	kJ/mol	Thermodynamic study of the sublimation of six halobenzoic acids
hsub	100.90 ± 0.50	kJ/mol	NIST Webbook
hsub	106.30 ± 0.50	kJ/mol	NIST Webbook
hsub	100.90 ± 0.50	kJ/mol	NIST Webbook
hvap	61.92	kJ/mol	Joback Method
log10ws	-1.89		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	413.45	K	Aqueous Solubility Prediction Method
tf	413.40 ± 0.30	K	NIST Webbook
tf	413.35	K	KDB
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.61	J/mol×K	574.70	Joback Method
cpg	221.19	J/mol×K	610.54	Joback Method
cpg	228.25	J/mol×K	646.38	Joback Method
cpg	234.81	J/mol×K	682.22	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
cps	163.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0001260	Pa×s	574.70	Joback Method
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	0.0041518	Pa×s	348.26	Joback Method
dvisc	0.0001839	Pa×s	536.96	Joback Method
dvisc	0.0002841	Pa×s	499.22	Joback Method
hfust	26.29	kJ/mol	414.10	NIST Webbook
hfust	25.25	kJ/mol	414.00	NIST Webbook
hfust	25.73	kJ/mol	413.40	NIST Webbook
hfust	25.73	kJ/mol	413.40	NIST Webbook
hfust	26.30	kJ/mol	414.00	NIST Webbook
hfust	25.73	kJ/mol	413.40	NIST Webbook
hsubt	105.00 ± 0.40	kJ/mol	329.50	NIST Webbook
hsubt	79.00 ± 2.00	kJ/mol	333.00	NIST Webbook
sfust	62.20	J/mol×K	413.40	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.81440e+01
Coeff. B	-9.09354e+03
Coeff. C	-1.04301e+02
Temperature range (K), min.	415.15
Temperature range (K), max.	502.57

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.35684e+02
Coeff. B	-1.50286e+04
Coeff. C	-1.67303e+01
Coeff. D	5.18960e-06
Temperature range (K), min.	415.15
Temperature range (K), max.	792.00

Sources

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

Thermodynamic study of the sublimation of six halobenzoic acids: https://www.doi.org/10.1016/j.jct.2004.09.005

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C118912&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1806

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1806

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
pvap:	Vapor 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