Benzoic acid, 5-chloro-2-hydroxy-

Other names:	Salicylic acid, 5-chloro-
	2-Hydroxy-5-chlorobenzoic acid
	5-Chloro-2-hydroxybenzoic acid
	5-Chlorosalicylic acid
	5 CSA
Inchi:	InChI=1S/C7H5ClO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,(H,10,11)
InchiKey:	NKBASRXWGAGQDP-UHFFFAOYSA-N
Formula:	C7H5ClO3
SMILES:	O=C(O)c1cc(Cl)ccc1O
Mol. weight [g/mol]:	172.57
CAS:	321-14-2

Physical Properties

Property code	Value	Unit	Source
gf	-321.45	kJ/mol	Joback Method
hf	-420.61	kJ/mol	Joback Method
hfus	23.21	kJ/mol	Joback Method
hvap	74.94	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.744		Crippen Method
mcvol	111.280	ml/mol	McGowan Method
pc	5853.95	kPa	Joback Method
rinpol	1480.00		NIST Webbook
tb	655.32	K	Joback Method
tc	879.90	K	Joback Method
tf	459.98	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.69	J/mol×K	655.32	Joback Method
cpg	256.05	J/mol×K	692.75	Joback Method
cpg	261.95	J/mol×K	730.18	Joback Method

cpg	267.47	J/mol×K	767.61	Joback Method
cpg	272.67	J/mol×K	805.04	Joback Method
cpg	277.63	J/mol×K	842.47	Joback Method
cpg	282.40	J/mol×K	879.90	Joback Method
dvisc	0.0004187	Pa×s	459.98	Joback Method
dvisc	0.0001872	Pa×s	492.54	Joback Method
dvisc	0.0000925	Pa×s	525.09	Joback Method
dvisc	0.0000496	Pa×s	557.65	Joback Method
dvisc	0.0000285	Pa×s	590.21	Joback Method
dvisc	0.0000174	Pa×s	622.76	Joback Method
dvisc	0.0000111	Pa×s	655.32	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C321142&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume