3-Chloro-4-hydroxybenzoic acid

Other names: Benzoic acid, 3-chloro-4-hydroxy-
Inchi: InChI=1S/C7H5ClO3/c8-5-3-4(7(10)11)1-2-6(5)9/h1-3,9H,(H,10,11)
InchiKey: QGNLHMKIGMZKJX-UHFFFAOYSA-N
Formula: C7H5ClO3
SMILES: O=C(O)c1ccc(O)c(Cl)c1
Mol. weight [g/mol]: 172.57
CAS: 3964-58-7

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
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

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=C3964587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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