3,5-Dichloro-4-hydroxybenzoic acid

Other names: Benzoic acid, 3,5-dichloro-4-hydroxy-
Inchi: InChI=1S/C7H4Cl2O3/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2,10H,(H,11,12)
InchiKey: AULKDLUOQCUNOK-UHFFFAOYSA-N
Formula: C7H4Cl2O3
SMILES: O=C(O)c1cc(Cl)c(O)c(Cl)c1
Mol. weight [g/mol]: 207.01
CAS: 3336-41-2

Physical Properties

Property code	Value	Unit	Source
gf	-343.01	kJ/mol	Joback Method
hf	-447.82	kJ/mol	Joback Method
hfus	27.01	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.397		Crippen Method
mcvol	123.520	ml/mol	McGowan Method
pc	5414.53	kPa	Joback Method
tb	697.73	K	Joback Method
tc	926.10	K	Joback Method
tf	502.42	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.58	J/mol×K	697.73	Joback Method
cpg	289.46	J/mol×K	888.04	Joback Method
cpg	284.93	J/mol×K	849.98	Joback Method
cpg	280.24	J/mol×K	811.92	Joback Method
cpg	275.33	J/mol×K	773.85	Joback Method
cpg	270.13	J/mol×K	735.79	Joback Method
cpg	293.90	J/mol×K	926.10	Joback Method
dvisc	0.0000077	Pa×s	697.73	Joback Method

dvisc	0.0000115	Pa×s	665.18	Joback Method
dvisc	0.0000179	Pa×s	632.63	Joback Method
dvisc	0.0000293	Pa×s	600.08	Joback Method
dvisc	0.0000506	Pa×s	567.52	Joback Method
dvisc	0.0000934	Pa×s	534.97	Joback Method
dvisc	0.0001867	Pa×s	502.42	Joback Method

Sources

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=C3336412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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