Benzoic acid, 3,6-dichloro-2-hydroxy

Other names: 3,6-dichlorosalicylic acid
Inchi: InChI=1S/C7H4Cl2O3/c8-3-1-2-4(9)6(10)5(3)7(11)12/h1-2,10H,(H,11,12)
InchiKey: FKIKPQHMWFZFEB-UHFFFAOYSA-N
Formula: C7H4Cl2O3
SMILES: O=C(O)c1c(Cl)ccc(Cl)c1O
Mol. weight [g/mol]: 207.01
CAS: 3401-80-7

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
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
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	270.13	J/mol×K	735.79	Joback Method
cpg	275.33	J/mol×K	773.85	Joback Method
cpg	280.24	J/mol×K	811.92	Joback Method
cpg	284.93	J/mol×K	849.98	Joback Method
cpg	289.46	J/mol×K	888.04	Joback Method

cpg	293.90	J/mol×K	926.10	Joback Method
dvisc	0.0001867	Pa×s	502.42	Joback Method
dvisc	0.0000934	Pa×s	534.97	Joback Method
dvisc	0.0000506	Pa×s	567.52	Joback Method
dvisc	0.0000293	Pa×s	600.08	Joback Method
dvisc	0.0000179	Pa×s	632.63	Joback Method
dvisc	0.0000115	Pa×s	665.18	Joback Method
dvisc	0.0000077	Pa×s	697.73	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3401807&Units=SI
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

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

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