Benzoic acid, 2,5-dichloro-3-hydroxy-6-methoxy-

Other names: o-Anisic acid, 3,6-dichloro-5-hydroxy-
5-Hydroxydicamba
3,6-Dichloro-5-hydroxy-2-methoxybenzoic acid
Inchi: InChI=1S/C8H6Cl2O4/c1-14-7-3(9)2-4(11)6(10)5(7)8(12)13/h2,11H,1H3,(H,12,13)
InchiKey: XYHBJALHMANCCC-UHFFFAOYSA-N
Formula: C8H6Cl2O4
SMILES: COc1c(Cl)cc(O)c(Cl)c1C(=O)O
Mol. weight [g/mol]: 237.04
CAS: 7600-50-2

Physical Properties

Property code	Value	Unit	Source
gf	-449.22	kJ/mol	Joback Method
hf	-612.15	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	85.28	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.406		Crippen Method
mcvol	143.480	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	748.01	K	Joback Method
tc	970.60	K	Joback Method
tf	410.35 ± 0.20	K	NIST Webbook
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.82	J/mol×K	748.01	Joback Method
cpg	337.37	J/mol×K	785.11	Joback Method
cpg	343.55	J/mol×K	822.21	Joback Method
cpg	349.43	J/mol×K	859.31	Joback Method
cpg	355.03	J/mol×K	896.40	Joback Method
cpg	360.40	J/mol×K	933.50	Joback Method

cpg	365.57	J/mol×K	970.60	Joback Method
dvisc	0.0000680	Pa×s	548.44	Joback Method
dvisc	0.0000368	Pa×s	581.70	Joback Method
dvisc	0.0000213	Pa×s	614.96	Joback Method
dvisc	0.0000130	Pa×s	648.23	Joback Method
dvisc	0.0000084	Pa×s	681.49	Joback Method
dvisc	0.0000056	Pa×s	714.75	Joback Method
dvisc	0.0000039	Pa×s	748.01	Joback Method
hfust	28.98	kJ/mol	409.80	NIST Webbook

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=C7600502&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
hfust: Enthalpy of fusion 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume