3,5-Diiodo-4-hydroxy-benzoic acid

Other names: 4-hydroxy-3,5-diiodobenzoic acid
Inchi: InChI=1S/C7H4I2O3/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2,10H,(H,11,12)
InchiKey: XREKTVACBXQCSB-UHFFFAOYSA-N
Formula: C7H4I2O3
SMILES: O=C(O)c1cc(I)c(O)c(I)c1
Mol. weight [g/mol]: 389.91
CAS: 618-76-8

Physical Properties

Property code	Value	Unit	Source
gf	-202.91	kJ/mol	Joback Method
hf	-262.60	kJ/mol	Joback Method
hfus	27.43	kJ/mol	Joback Method
hvap	89.96	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.300		Crippen Method
mcvol	150.680	ml/mol	McGowan Method
pc	5661.74	kPa	Joback Method
tb	809.15	K	Joback Method
tc	1079.41	K	Joback Method
tf	558.70	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.46	J/mol×K	809.15	Joback Method
cpg	287.54	J/mol×K	854.19	Joback Method
cpg	292.57	J/mol×K	899.24	Joback Method
cpg	297.67	J/mol×K	944.28	Joback Method
cpg	303.00	J/mol×K	989.32	Joback Method
cpg	308.70	J/mol×K	1034.37	Joback Method
cpg	314.91	J/mol×K	1079.41	Joback Method
dvisc	0.0000951	Pa×s	558.70	Joback Method

dvisc	0.0000446	Pa×s	600.44	Joback Method
dvisc	0.0000230	Pa×s	642.18	Joback Method
dvisc	0.0000129	Pa×s	683.92	Joback Method
dvisc	0.0000077	Pa×s	725.67	Joback Method
dvisc	0.0000049	Pa×s	767.41	Joback Method
dvisc	0.0000033	Pa×s	809.15	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=C618768&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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