Benzoic acid, 2-hydroxy-3,5-diiodo-

Other names:	2-Hydroxy-3,5-diiodobenzenecarboxylic acid
	2-Hydroxy-3,5-diiodobenzoate
	2-Hydroxy-3,5-diiodobenzoic acid
	3,5-Diiodo-2-hydroxybenzoic acid
	3,5-Diiodosalicylic acid
	Benzoic acid, 3,5-diiodo-2-hydroxy-
	NSC 6303
	Salicylic acid, 3,5-diiodo-
Inchi:	InChI=1S/C7H4I2O3/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2,10H,(H,11,12)
InchiKey:	DHZVWQPHNWDCFS-UHFFFAOYSA-N
Formula:	C7H4I2O3
SMILES:	O=C(O)c1cc(I)cc(I)c1O
Mol. weight [g/mol]:	389.91
CAS:	133-91-5

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	-3.31		Aqueous Solubility Prediction 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	506.40	K	Aqueous Solubility Prediction 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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C133915&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