Benzoic acid, 5-bromo-2-hydroxy-

Other names:	Salicylic acid, 5-bromo-
	2-Hydroxy-5-bromobenzoic acid
	5-Bromo-2-hydroxybenzoic acid
	5-Bromosalicylic acid
	Benzoic acid, 3-bromo-6-hydroxy-
Inchi:	InChI=1S/C7H5BrO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,(H,10,11)
InchiKey:	IEJOONSLOGAXNO-UHFFFAOYSA-N
Formula:	C7H5BrO3
SMILES:	O=C(O)c1cc(Br)ccc1O
Mol. weight [g/mol]:	217.02
CAS:	89-55-4

Physical Properties

Property code	Value	Unit	Source
gf	-295.20	kJ/mol	Joback Method
hf	-378.54	kJ/mol	Joback Method
hfus	24.29	kJ/mol	Joback Method
hvap	76.99	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.853		Crippen Method
mcvol	116.540	ml/mol	McGowan Method
pc	6932.88	kPa	Joback Method
tb	684.05	K	Joback Method
tc	916.63	K	Joback Method
tf	489.86	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.56	J/mol×K	684.05	Joback Method
cpg	282.69	J/mol×K	877.87	Joback Method
cpg	277.76	J/mol×K	839.11	Joback Method
cpg	272.67	J/mol×K	800.34	Joback Method

cpg	267.33	J/mol×K	761.58	Joback Method
cpg	261.65	J/mol×K	722.81	Joback Method
cpg	287.53	J/mol×K	916.63	Joback Method
dvisc	0.0000092	Pa×s	684.05	Joback Method
dvisc	0.0000139	Pa×s	651.69	Joback Method
dvisc	0.0000220	Pa×s	619.32	Joback Method
dvisc	0.0000366	Pa×s	586.96	Joback Method
dvisc	0.0000647	Pa×s	554.59	Joback Method
dvisc	0.0001225	Pa×s	522.23	Joback Method
dvisc	0.0002524	Pa×s	489.86	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C89554&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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