

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/molxK	684.05	Joback Method
cpg	282.69	J/molxK	877.87	Joback Method
cpg	277.76	J/molxK	839.11	Joback Method
cpg	272.67	J/molxK	800.34	Joback Method

cpg	267.33	J/molxK	761.58	Joback Method
cpg	261.65	J/molxK	722.81	Joback Method
cpg	287.53	J/molxK	916.63	Joback Method
dvisc	0.0000092	Paxs	684.05	Joback Method
dvisc	0.0000139	Paxs	651.69	Joback Method
dvisc	0.0000220	Paxs	619.32	Joback Method
dvisc	0.0000366	Paxs	586.96	Joback Method
dvisc	0.0000647	Paxs	554.59	Joback Method
dvisc	0.0001225	Paxs	522.23	Joback Method
dvisc	0.0002524	Paxs	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/ci9903071
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

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