

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

Other names:	Salicylic acid, 3,5-dibromo- 2-Hydroxy-3,5-dibromobenzoic acid 3,5-Dibromo-2-hydroxybenzoic acid 3,5-Dibromosalicylic acid
Inchi:	InChI=1S/C7H4Br2O3/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2,10H,(H,11,12)
InchiKey:	BFBZHSOXXKROMBG-UHFFFAOYSA-N
Formula:	C7H4Br2O3
SMILES:	O=C(O)c1cc(Br)cc(Br)c1O
Mol. weight [g/mol]:	295.91
CAS:	3147-55-5

Physical Properties

Property code	Value	Unit	Source
gf	-290.51	kJ/mol	Joback Method
hf	-363.68	kJ/mol	Joback Method
hfus	29.19	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.615		Crippen Method
mcvol	134.040	ml/mol	McGowan Method
pc	7601.04	kPa	Joback Method
tb	755.19	K	Joback Method
tc	998.68	K	Joback Method
tf	562.18	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.30	J/molxK	755.19	Joback Method
cpg	298.90	J/molxK	958.09	Joback Method
cpg	294.03	J/molxK	917.51	Joback Method
cpg	289.23	J/molxK	876.93	Joback Method
cpg	284.41	J/molxK	836.35	Joback Method

cpg	279.47	J/molxK	795.77	Joback Method
cpg	303.94	J/molxK	998.68	Joback Method
dvisc	0.0000051	Paxs	755.19	Joback Method
dvisc	0.0000072	Paxs	723.02	Joback Method
dvisc	0.0000106	Paxs	690.85	Joback Method
dvisc	0.0000161	Paxs	658.68	Joback Method
dvisc	0.0000257	Paxs	626.52	Joback Method
dvisc	0.0000429	Paxs	594.35	Joback Method
dvisc	0.0000761	Paxs	562.18	Joback Method

Sources

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=C3147555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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