3,5-Dibromo-4-hydroxybenzoic acid

Other names:	Benzoic acid, 3,5-dibromo-4-hydroxy- Bromoxynylbenzoic acid
Inchi:	InChI=1S/C7H4Br2O3/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2,10H,(H,11,12)
InchiKey:	PHWAJJWKNLWZGJ-UHFFFAOYSA-N
Formula:	C7H4Br2O3
SMILES:	O=C(O)c1cc(Br)c(O)c(Br)c1
Mol. weight [g/mol]:	295.91
CAS:	3337-62-0

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/mol×K	755.19	Joback Method
cpg	298.90	J/mol×K	958.09	Joback Method
cpg	294.03	J/mol×K	917.51	Joback Method
cpg	289.23	J/mol×K	876.93	Joback Method
cpg	284.41	J/mol×K	836.35	Joback Method
cpg	279.47	J/mol×K	795.77	Joback Method
cpg	303.94	J/mol×K	998.68	Joback Method

dvisc	0.0000051	Pa×s	755.19	Joback Method
dvisc	0.0000072	Pa×s	723.02	Joback Method
dvisc	0.0000106	Pa×s	690.85	Joback Method
dvisc	0.0000161	Pa×s	658.68	Joback Method
dvisc	0.0000257	Pa×s	626.52	Joback Method
dvisc	0.0000429	Pa×s	594.35	Joback Method
dvisc	0.0000761	Pa×s	562.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3337620&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