5-Bromo-2,4-dihydroxybenzoic acid

Other names:	2,4-Dihydroxy-5-bromobenzoic acid 5-Bromo-«beta»-resorcylic acid 5-Bromo-Â«betaÂ»-resorcylic acid Benzoic acid, 5-bromo-2,4-dihydroxy- diphenylhydantoin «beta»-Resorcylic acid, 5-bromo- Â«betaÂ»-Resorcylic acid, 5-bromo-
Inchi:	InChI=1S/C7H5BrO4/c8-4-1-3(7(11)12)5(9)2-6(4)10/h1-2,9-10H,(H,11,12)
InchiKey:	ZRBCISXJLHZOMS-UHFFFAOYSA-N
Formula:	C7H5BrO4
SMILES:	O=C(O)c1cc(Br)c(O)cc1O
Mol. weight [g/mol]:	233.02
CAS:	7355-22-8

Physical Properties

Property code	Value	Unit	Source
gf	-449.82	kJ/mol	Joback Method
hf	-555.85	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	90.00	kJ/mol	Joback Method
log10ws	-3.86		Aqueous Solubility Prediction Method
logp	1.558		Crippen Method
mcvol	122.410	ml/mol	McGowan Method
pc	9035.84	kPa	Joback Method
tb	764.67	K	Joback Method
tc	1004.37	K	Joback Method
tf	601.58	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.67	J/mol×K	764.67	Joback Method

cpg	292.08	J/mol×K	804.62	Joback Method
cpg	297.43	J/mol×K	844.57	Joback Method
cpg	302.89	J/mol×K	884.52	Joback Method
cpg	308.58	J/mol×K	924.47	Joback Method
cpg	314.65	J/mol×K	964.42	Joback Method
cpg	321.25	J/mol×K	1004.37	Joback Method
dvisc	0.0000068	Pa×s	601.58	Joback Method
dvisc	0.0000037	Pa×s	628.76	Joback Method
dvisc	0.0000022	Pa×s	655.94	Joback Method
dvisc	0.0000013	Pa×s	683.12	Joback Method
dvisc	0.0000008	Pa×s	710.31	Joback Method
dvisc	0.0000005	Pa×s	737.49	Joback Method
dvisc	0.0000004	Pa×s	764.67	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7355228&Units=SI

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

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