Benzaldehyde, 5-bromo-2-hydroxy-

Other names:	5-Bromo-2-hydroxybenzaldehyde
	5-Bromosalicylaldehyde
	2-Hydroxy-5-bromobenzaldehyde
	Salicylaldehyde, 5-bromo-
	5-Bromo-salicyclaldehyde
Inchi:	InChI=1S/C7H5BrO2/c8-6-1-2-7(10)5(3-6)4-9/h1-4,10H
InchiKey:	MKKSTJKBKNCMRV-UHFFFAOYSA-N
Formula:	C7H5BrO2
SMILES:	O=Cc1cc(Br)ccc1O
Mol. weight [g/mol]:	201.02
CAS:	1761-61-1

Physical Properties

Property code	Value	Unit	Source
gf	-128.98	kJ/mol	Joback Method
hf	-199.31	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	60.28	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.967		Crippen Method
mcvol	110.670	ml/mol	McGowan Method
pc	6084.49	kPa	Joback Method
tb	586.66	K	Joback Method
tc	836.48	K	Joback Method
tf	421.11	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.99	J/mol×K	586.66	Joback Method
cpg	256.02	J/mol×K	794.84	Joback Method
cpg	250.54	J/mol×K	753.21	Joback Method
cpg	244.71	J/mol×K	711.57	Joback Method

cpg	238.40	J/mol×K	669.93	Joback Method
cpg	231.53	J/mol×K	628.30	Joback Method
cpg	261.23	J/mol×K	836.48	Joback Method
dvisc	0.0000668	Pa×s	586.66	Joback Method
dvisc	0.0000930	Pa×s	559.07	Joback Method
dvisc	0.0001341	Pa×s	531.48	Joback Method
dvisc	0.0002013	Pa×s	503.88	Joback Method
dvisc	0.0003168	Pa×s	476.29	Joback Method
dvisc	0.0005269	Pa×s	448.70	Joback Method
dvisc	0.0009370	Pa×s	421.11	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1761611&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

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