

Benzaldehyde, 5-bromo-2-hydroxy-

Other names:	5-Bromo-2-hydroxybenzaldehyde 5-Bromosalicylaldehyde 2-Hydroxy-5-bromobenzaldehyde Salicylaldehyde, 5-bromo- 5-Bromo-salicylaldehyde
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/molxK	586.66	Joback Method
cpg	231.53	J/molxK	628.30	Joback Method
cpg	238.40	J/molxK	669.93	Joback Method
cpg	244.71	J/molxK	711.57	Joback Method

cpg	250.54	J/molxK	753.21	Joback Method
cpg	256.02	J/molxK	794.84	Joback Method
cpg	261.23	J/molxK	836.48	Joback Method
dvisc	0.0009370	Paxs	421.11	Joback Method
dvisc	0.0005269	Paxs	448.70	Joback Method
dvisc	0.0003168	Paxs	476.29	Joback Method
dvisc	0.0002013	Paxs	503.88	Joback Method
dvisc	0.0001341	Paxs	531.48	Joback Method
dvisc	0.0000930	Paxs	559.07	Joback Method
dvisc	0.0000668	Paxs	586.66	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=C1761611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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