Benzaldehyde, 3-bromo-4-hydroxy-

Other names:	3-Bromo-4-hydroxybenzaldehyde
	4-Hydroxy-3-bromobenzaldehyde
Inchi:	InChI=1S/C7H5BrO2/c8-6-3-5(4-9)1-2-7(6)10/h1-4,10H
InchiKey:	UOTMHAOCAJROQF-UHFFFAOYSA-N
Formula:	C7H5BrO2
SMILES:	O=Cc1ccc(O)c(Br)c1
Mol. weight [g/mol]:	201.02
CAS:	2973-78-6

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	-2.18		Aqueous Solubility Prediction 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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2973786&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