

3-Bromo-5-chloro-2-hydroxybenzaldehyde

Other names:	Benzaldehyde, 3-bromo-5-chloro-2-hydroxy-
Inchi:	InChI=1S/C7H4BrClO2/c8-6-2-5(9)1-4(3-10)7(6)11/h1-3,11H
InchiKey:	KNOYZLVIXXBBIB-UHFFFAOYSA-N
Formula:	C7H4BrClO2
SMILES:	O=Cc1cc(Cl)cc(Br)c1O
Mol. weight [g/mol]:	235.46
CAS:	19652-32-5

Physical Properties

Property code	Value	Unit	Source
gf	-150.54	kJ/mol	Joback Method
hf	-226.52	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	65.33	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.621		Crippen Method
mcvol	122.910	ml/mol	McGowan Method
pc	5619.38	kPa	Joback Method
tb	629.07	K	Joback Method
tc	883.09	K	Joback Method
tf	463.55	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.20	J/mol×K	629.07	Joback Method
cpg	246.65	J/mol×K	671.41	Joback Method
cpg	252.57	J/mol×K	713.74	Joback Method
cpg	258.07	J/mol×K	756.08	Joback Method
cpg	263.23	J/mol×K	798.42	Joback Method
cpg	268.16	J/mol×K	840.76	Joback Method
cpg	272.96	J/mol×K	883.09	Joback Method
dvisc	0.0004941	Pa×s	463.55	Joback Method

dvisc	0.0003021	Pa×s	491.14	Joback Method
dvisc	0.0001946	Pa×s	518.72	Joback Method
dvisc	0.0001310	Pa×s	546.31	Joback Method
dvisc	0.0000916	Pa×s	573.90	Joback Method
dvisc	0.0000662	Pa×s	601.48	Joback Method
dvisc	0.0000493	Pa×s	629.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19652325&Units=SI

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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