3-Bromo-2-hydroxy-5-nitrobenzaldehyde

Inchi: InChI=1S/C7H4BrNO4/c8-6-2-5(9(12)13)1-4(3-10)7(6)11/h1-3,11H
InchiKey: BESBCGANGAEHPM-UHFFFAOYSA-N
Formula: C7H4BrNO4
SMILES: O=Cc1cc([N+](=O)[O-])cc(Br)c1O
Mol. weight [g/mol]: 246.01
CAS: 16789-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-103.06	kJ/mol	Joback Method
hf	-221.54	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	77.54	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	1.875		Crippen Method
mcvol	128.090	ml/mol	McGowan Method
pc	6056.11	kPa	Joback Method
tb	743.48	K	Joback Method
tc	1014.70	K	Joback Method
tf	577.24	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.26	J/mol×K	743.48	Joback Method
cpg	296.88	J/mol×K	788.68	Joback Method
cpg	303.09	J/mol×K	833.89	Joback Method
cpg	308.99	J/mol×K	879.09	Joback Method
cpg	314.74	J/mol×K	924.30	Joback Method
cpg	320.46	J/mol×K	969.50	Joback Method
cpg	326.27	J/mol×K	1014.70	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=C16789847&Units=SI

Legend

cpg:	Ideal gas heat capacity
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