2-Bromobenzaldoxime

Other names: Benzaldehyde, 2-bromo-, oxime
Inchi: InChI=1S/C7H6BrNO/c8-7-4-2-1-3-6(7)5-9-10/h1-5,10H
InchiKey: PSIRFUPZHPEKAE-UHFFFAOYSA-N
Formula: C7H6BrNO
SMILES: ON=Cc1ccccc1Br
Mol. weight [g/mol]: 200.03
CAS: 34158-72-0

Physical Properties

Property code	Value	Unit	Source
hf	-6.43	kJ/mol	Joback Method
hvap	60.54	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	2.257		Crippen Method
mcvol	114.780	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	626.24	K	Joback Method
tc	858.33	K	Joback Method

Sources

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=C34158720&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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

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