

3-Bromophenyl isocyanate

Inchi: InChI=1S/C7H4BrNO/c8-6-2-1-3-7(4-6)9-5-10/h1-4H
InchiKey: VQVBCZQTXSHJGF-UHFFFAOYSA-N
Formula: C7H4BrNO
SMILES: O=C=Nc1cccc(Br)c1
Mol. weight [g/mol]: 198.02
CAS: 23138-55-8

Physical Properties

Property code	Value	Unit	Source
hf	58.17	kJ/mol	Joback Method
hvap	50.08	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	2.416		Crippen Method
mcvol	110.480	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	524.05	K	Joback Method
tc	766.95	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23138558&Units=SI>
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

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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