

2-Bromophenyl isocyanate

Inchi:	InChI=1S/C7H4BrNO/c8-6-3-1-2-4-7(6)9-5-10/h1-4H
InchiKey:	GOOVAYJIVMBWPP-UHFFFAOYSA-N
Formula:	C7H4BrNO
SMILES:	O=C=Nc1ccccc1Br
Mol. weight [g/mol]:	198.02
CAS:	1592-00-3

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1592003&Units=SI

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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