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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1592003&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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