Quinoline, 3-bromo-

Other names: 3-Bromoquinoline
Inchi: InChI=1S/C9H6BrN/c10-8-5-7-3-1-2-4-9(7)11-6-8/h1-6H
InchiKey: ZGIKWINFUGEQEO-UHFFFAOYSA-N
Formula: C9H6BrN
SMILES: Brc1cnc2ccccc2c1
Mol. weight [g/mol]: 208.06
CAS: 5332-24-1

Physical Properties

Property code	Value	Unit	Source
hvap	70.70 ± 2.30	kJ/mol	NIST Webbook
log10ws	-4.20		Crippen Method
logp	2.997		Crippen Method
mcvol	121.930	ml/mol	McGowan Method
rinpol	1452.20		NIST Webbook
tb	548.20	K	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5332241&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature