Quinoline, 6-bromo-

Other names: 6-Bromoquinoline
Inchi: InChI=1S/C9H6BrN/c10-8-3-4-9-7(6-8)2-1-5-11-9/h1-6H
InchiKey: IFIHYLCUKYCKRH-UHFFFAOYSA-N
Formula: C9H6BrN
SMILES: Brc1ccc2ncccc2c1
Mol. weight [g/mol]: 208.06
CAS: 5332-25-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	2.997		Crippen Method
mcvol	121.930	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5332252&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume