

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

Latest version available from:

<https://www.chemeo.com/cid/26-212-7/Quinoline-6-bromo.pdf>

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