

7-bromoquinoline

Inchi:	InChI=1S/C9H6BrN/c10-8-4-3-7-2-1-5-11-9(7)6-8/h1-6H
InchiKey:	XYBSZCUHOLWQQU-UHFFFAOYSA-N
Formula:	C9H6BrN
SMILES:	Brc1ccc2cccnc2c1
Mol. weight [g/mol]:	208.06
CAS:	4965-36-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	2.997		Crippen Method
mcvol	121.930	ml/mol	McGowan Method
tf	308.00 ± 2.00	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4965360&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/108-354-9/7-bromoquinoline.pdf>

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