

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/ci9903071
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

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<https://www.chemeo.com/cid/27-879-7/Quinoline-3-bromo.pdf>

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