

# Isoquinoline, 4-bromo-

<b>Other names:</b>	4-Bromoisquinoline
<b>Inchi:</b>	InChI=1S/C9H6BrN/c10-9-6-11-5-7-3-1-2-4-8(7)9/h1-6H
<b>InchiKey:</b>	SCRBSGZBTHKAHU-UHFFFAOYSA-N
<b>Formula:</b>	C9H6BrN
<b>SMILES:</b>	Brc1cncc2ccccc12
<b>Mol. weight [g/mol]:</b>	208.06
<b>CAS:</b>	1532-97-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	2.997		Crippen Method
mcvol	121.930	ml/mol	McGowan Method
tb	555.70	K	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1532974&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1532974&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tb:</b>	Normal Boiling Point Temperature

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