

# Quinoxaline, 2-(tribromomethyl)-

<b>Inchi:</b>	InChI=1S/C9H5Br3N2/c10-9(11,12)8-5-13-6-3-1-2-4-7(6)14-8/h1-5H
<b>InchiKey:</b>	VCCOPRMZNNMFLI-UHFFFAOYSA-N
<b>Formula:</b>	C9H5Br3N2
<b>SMILES:</b>	BrC(Br)(Br)c1cnc2cccc2n1
<b>Mol. weight [g/mol]:</b>	380.86
<b>CAS:</b>	7251-36-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.65		Crippen Method
logp	3.925		Crippen Method
mcvol	166.910	ml/mol	McGowan Method

## Sources

<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=C7251367&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7251367&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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

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<https://www.chemeo.com/cid/22-966-5/Quinoxaline-2-tribromomethyl.pdf>

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