

2-Methyl-5,6,7,8-tetrahydroquinoxaline

Inchi:	InChI=1S/C9H12N2/c1-7-6-10-8-4-2-3-5-9(8)11-7/h6H,2-5H2,1H3
InchiKey:	JSAHYTOSTYPIJ-UHFFFAOYSA-N
Formula:	C9H12N2
SMILES:	Cc1cnc2c(n1)CCCC2
Mol. weight [g/mol]:	148.21
CAS:	38917-65-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	1.664		Crippen Method
mcvol	123.010	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38917656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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