

N-Methylhomopiperazine

Other names:	1H-1,4-Diazepine, hexahydro-1-methyl-
Inchi:	InChI=1S/C6H14N2/c1-8-5-2-3-7-4-6-8/h7H,2-6H2,1H3
InchiKey:	FXHRAKUEZPSMLJ-UHFFFAOYSA-N
Formula:	C6H14N2
SMILES:	CN1CCCNCC1
Mol. weight [g/mol]:	114.19
CAS:	4318-37-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.01		Crippen Method
logp	-0.088		Crippen Method
mcvol	104.500	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=C4318370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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