

1,3-Dimethyltetrahydro-2(1H)pyrimidine

Inchi:	InChI=1S/C6H12N2/c1-7-4-3-5-8(2)6-7/h3-4H,5-6H2,1-2H3
InchiKey:	UPCMWHVBPPBFPF-UHFFFAOYSA-N
Formula:	C6H12N2
SMILES:	CN1C=CCN(C)C1
Mol. weight [g/mol]:	112.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.21		Crippen Method
logp	0.335		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
rmpol	1007.00		NIST Webbook
rmpol	1010.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R588526&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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