

# 3H-1,4-benzodiazepine, 1,2,4,5-tetrahydro-4-(p-methoxyphenyl)-1-methyl-

Inchi:	InChI=1S/C17H20N2O/c1-18-11-12-19(13-14-5-3-4-6-17(14)18)15-7-9-16(20-2)10-8-15/
InchiKey:	DJSNZUDEZGVXCG-UHFFFAOYSA-N
Formula:	C17H20N2O
SMILES:	COc1ccc(N2CCN(C)c3ccccc3C2)cc1
Mol. weight [g/mol]:	268.35
CAS:	1033-18-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	3.152		Crippen Method
mcvol	217.840	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1033187&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1033187&amp;Units=SI</a>

## Legend

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

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