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/l

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: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.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=C1033187&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume