

3H-1,4-benzodiazepine-2,5-dione, 1,2,4,5-tetrahydro-1-methyl-4-phenyl-

Inchi:	InChI=1S/C16H14N2O2/c1-17-14-10-6-5-9-13(14)16(20)18(11-15(17)19)12-7-3-2-4-8-12
InchiKey:	NULVUNPOPBZGBZ-UHFFFAOYSA-N
Formula:	C16H14N2O2
SMILES:	CN1C(=O)CN(c2ccccc2)C(=O)c2ccccc21
Mol. weight [g/mol]:	266.29
CAS:	1032-21-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	2.310		Crippen Method
mcvol	201.020	ml/mol	McGowan Method

Sources

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=C1032219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/21-454-4/3H-1-4-benzodiazepine-2-5-dione-1-2-4-5-tetrahydro-1-methyl-4-phenyl.pdf>

Generated by Cheméo on 2025-12-22 01:31:18.426082163 +0000 UTC m=+6115275.956122818.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.