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