3-Methyl-1-benzoyl-(1H)-1,2-diazepine

Inchi: InChI=1S/C13H12N2O/c1-11-7-5-6-10-15(14-11)13(16)12-8-3-2-4-9-12/h2-10H,1H3
InchiKey: PHQSCYFZZWMASY-UHFFFAOYSA-N
Formula: C13H12N2O
SMILES: CC1=NN(C(=O)c2ccccc2)C=CC=C1
Mol. weight [g/mol]: 212.25
CAS: 69298-66-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	2.588		Crippen Method
mcvol	168.040	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=C69298664&Units=SI

Legend

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