

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

Inchi:	InChI=1S/C13H12N2O/c1-11-7-9-14-15(10-8-11)13(16)12-5-3-2-4-6-12/h2-10H,1H3
InchiKey:	WZZSZCWZNUBGAN-UHFFFAOYSA-N
Formula:	C13H12N2O
SMILES:	CC1=CC=NN(C(=O)c2ccccc2)C=C1
Mol. weight [g/mol]:	212.25
CAS:	64762-45-4

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/ci9903071
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=C64762454&Units=SI

Legend

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

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