

1-Phenyl-1,3,8-triazaspiro[4.5]decan-4-one

Other names:	1,3,8-Triazaspiro[4.5]decan-4-one, 1-phenyl-1-Phenyl-1,3,8-triazaspiro[4,5]decan-4-one
Inchi:	InChI=1S/C13H17N3O/c17-12-13(6-8-14-9-7-13)16(10-15-12)11-4-2-1-3-5-11/h1-5,14H,
InchiKey:	HTQWGIHCFPWKAS-UHFFFAOYSA-N
Formula:	C13H17N3O
SMILES:	O=C1NCN(c2ccccc2)C12CCNCC2
Mol. weight [g/mol]:	231.29
CAS:	1021-25-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	0.702		Crippen Method
mcvol	180.060	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1021256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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