

# Oxolamine

<b>Other names:</b>	1,2,4-Oxadiazole-5-ethanamine, N,N-diethyl-3-phenyl- 1,2,4-Oxadiazole, 5-(2-(diethylamino)ethyl)-3-phenyl- AF 438 5-(2-Diethylaminoethyl)-3-phenyl-1,2,4-oxadiazole N,N-Diethyl-3-phenyl-1,2,4-oxadiazole-5-ethanamine 5-(2-Diethylaminoethyl)-3-phenyl-1,2,4-oxadiazole 683 M Oxolamina 3-Phenyl-5-(«beta»-diethylaminoethyl)-1,2,4-oxadiazole
<b>Inchi:</b>	InChI=1S/C14H19N3O/c1-3-17(4-2)11-10-13-15-14(16-18-13)12-8-6-5-7-9-12/h5-9H,3-4
<b>InchiKey:</b>	IDCHQQSVJAAUQQ-UHFFFAOYSA-N
<b>Formula:</b>	C14H19N3O
<b>SMILES:</b>	CCN(CC)CCc1nc(-c2ccccc2)no1
<b>Mol. weight [g/mol]:</b>	245.32
<b>CAS:</b>	959-14-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.39		Crippen Method
logp	2.621		Crippen Method
mcvol	200.710	ml/mol	McGowan Method
rinpol	1869.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C959148&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C959148&amp;Units=SI</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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