

# 2-(1-Naphthyl)-5-phenyl-1,3,4-oxadiazole

<b>Other names:</b>	«alpha»-NPD 1,3,4-Oxadiazole, 2-(1-naphthalenyl)-5-phenyl- 1,3,4-Oxadiazole, 2-(1-naphthyl)-5-phenyl-
<b>Inchi:</b>	InChI=1S/C18H12N2O/c1-2-8-14(9-3-1)17-19-20-18(21-17)16-12-6-10-13-7-4-5-11-15(1)
<b>InchiKey:</b>	PNPLRTWSLDSFET-UHFFFAOYSA-N
<b>Formula:</b>	C18H12N2O
<b>SMILES:</b>	<chem>c1ccc(-c2nnc(-c3cccc4ccccc34)o2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	272.30
<b>CAS:</b>	897-18-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-11.75		Crippen Method
logp	4.557		Crippen Method
mcvol	203.870	ml/mol	McGowan Method

## Sources

<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=C897187&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C897187&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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

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