

2-Phenyl-4-methyl-oxadiazol-1,3,4-one-5

Other names:	1,3,4 Oxadiazol-2(3H)-one, 3-methyl-5-phenyl
Inchi:	InChI=1S/C9H8N2O2/c1-11-9(12)13-8(10-11)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	JBDTUVFVJKCGHG-UHFFFAOYSA-N
Formula:	C9H8N2O2
SMILES:	Cn1nc(-c2ccccc2)oc1=O
Mol. weight [g/mol]:	176.17
CAS:	879-60-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.28		Crippen Method
logp	1.040		Crippen Method
mcvol	126.150	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=C879607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:

<https://www.chemeo.com/cid/45-456-6/2-Phenyl-4-methyl-oxadiazol-1-3-4-one-5.pdf>

Generated by Cheméo on 2024-07-18 03:39:10.417882268 +0000 UTC m=+500165.613852644.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.