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