

1,2,4-Oxadiazole, 3-methyl-5-phenyl-

Other names:	3-Methyl-5-phenyl-1,2,4-oxadiazole
Inchi:	InChI=1S/C9H8N2O/c1-7-10-9(12-11-7)8-5-3-2-4-6-8/h2-6H,1H3
InchiKey:	ZTWRWSTUMWZTAU-UHFFFAOYSA-N
Formula:	C9H8N2O
SMILES:	Cc1noc(-c2ccccc2)n1
Mol. weight [g/mol]:	160.17
CAS:	1199-00-4

Physical Properties

Property code	Value	Unit	Source
chs	-4788.20 ± 5.40	kJ/mol	NIST Webbook
log10ws	-7.82		Crippen Method
logp	2.045		Crippen Method
mcvol	120.280	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1199004&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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