

1,3,4-Oxadiazol-2(3h)-one, 3-acetyl-5-(5-nitro-2-furyl)-

Inchi:	InChI=1S/C8H5N3O6/c1-4(12)10-8(13)17-7(9-10)5-2-3-6(16-5)11(14)15/h2-3H,1H3
InchiKey:	NLAXZJRCPGWATL-UHFFFAOYSA-N
Formula:	C8H5N3O6
SMILES:	CC(=O)n1nc(-c2ccc([N+](=O)[O-])o2)oc1=O
Mol. weight [g/mol]:	239.14
CAS:	116401-76-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.50		Crippen Method
logp	0.665		Crippen Method
mcvol	141.220	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401764&Units=SI

Legend

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

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