

Oxadiazole, 1,3,4-, 2-methylthio-5-(5-nitro-2-furyl)-

Inchi:	InChI=1S/C7H5N3O4S/c1-15-7-9-8-6(14-7)4-2-3-5(13-4)10(11)12/h2-3H,1H3
InchiKey:	RLLLGECDCWMELF-UHFFFAOYSA-N
Formula:	C7H5N3O4S
SMILES:	CSc1nnc(-c2ccc([N+](=O)[O-])o2)o1
Mol. weight [g/mol]:	227.20
CAS:	98273-49-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.47		Crippen Method
logp	1.960		Crippen Method
mcvol	136.040	ml/mol	McGowan Method

Sources

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=C98273495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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