

Oxadiazole, 1,2,4-, 3-(5-nitrofuran-2-yl)-5-(phenyloxymethyl)-

Inchi:	InChI=1S/C13H9N3O5/c17-16(18)12-7-6-10(20-12)13-14-11(21-15-13)8-19-9-4-2-1-3-5-
InchiKey:	LUMWKTIGOPJHGW-UHFFFAOYSA-N
Formula:	C13H9N3O5
SMILES:	O=[N+]([O-])c1ccc(-c2noc(COc3ccccc3)n2)o1
Mol. weight [g/mol]:	287.23
CAS:	36883-92-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.95		Crippen Method
logp	2.817		Crippen Method
mcvol	186.340	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=C36883928&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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