

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

Inchi:	InChI=1S/C11H12N4O5/c16-15(17)10-2-1-8(19-10)11-12-9(13-20-11)7-14-3-5-18-6-4-14
InchiKey:	FOPOXQKKPMUWFM-UHFFFAOYSA-N
Formula:	C11H12N4O5
SMILES:	O=[N+]([O-])c1ccc(-c2nc(CN3CCOCC3)no2)o1
Mol. weight [g/mol]:	280.24
CAS:	36133-75-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.83		Crippen Method
logp	1.070		Crippen Method
mcvol	181.040	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=C36133752&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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