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

Inchi: InChI=1S/C11H6N4O4/c16-15(17)9-2-1-8(18-9)11-13-10(14-19-11)7-3-5-12-6-4-7/h1-6H

InchiKey: VABZRAFKJLBBMK-UHFFFAOYSA-N

Formula: C11H6N4O4

SMILES: O=[N+]([O-])c1ccc(-c2nc(-c3ccncc3)no2)o1

Mol. weight [g/mol]: 258.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.09		Crippen Method
logp	2.300		Crippen Method
mcvol	162.270	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009059&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume