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

Inchi: InChI=1S/C7H4ClN3O4/c8-3-5-9-7(15-10-5)4-1-2-6(14-4)11(12)13/h1-2H,3H2
InchiKey: FFEGRFNTSRKNIR-UHFFFAOYSA-N
Formula: C7H4ClN3O4
SMILES: O=[N+]([O-])c1ccc(-c2nc(CCl)no2)o1
Mol. weight [g/mol]: 229.58
CAS: 129206-53-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.76		Crippen Method
logp	1.977		Crippen Method
mcvol	131.930	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=C129206537&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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