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

Inchi: InChI=1S/C7H3Cl2N3O4/c8-5(9)7-10-6(11-16-7)3-1-2-4(15-3)12(13)14/h1-2,5H
InchiKey: POPKILWDQYTNSY-UHFFFAOYSA-N
Formula: C7H3Cl2N3O4
SMILES: O=[N+]([O-])c1ccc(-c2noc(C(Cl)Cl)n2)o1
Mol. weight [g/mol]: 264.02
CAS: 5671-14-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.37		Crippen Method
logp	2.714		Crippen Method
mcvol	144.170	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=C5671147&Units=SI

Legend

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