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

Inchi: InChI=1S/C12H6ClN3O4/c13-8-3-1-2-7(6-8)12-14-11(15-20-12)9-4-5-10(19-9)16(17)18/h

InchiKey: DUQRWENEUUABMM-UHFFFAOYSA-N

Formula: C12H6ClN3O4

SMILES: O=[N+]([O-])c1ccc(-c2noc(-c3cccc(Cl)c3)n2)o1

Mol. weight [g/mol]: 291.65

CAS: 5671-09-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.01		Crippen Method
logp	3.558		Crippen Method
mcvol	178.620	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5671090&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/75-376-2/Oxadiazole-1-2-4-5-3-chlorophenyl-3-5-nitrofuran-2-yl.pdf
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