

Oxadiazole, 1,2,4-, 3-chloromethyl-5-(5-nitrofur-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

Latest version available from:

<https://www.chemeo.com/cid/27-029-0/Oxadiazole-1-2-4-3-chloromethyl-5-5-nitrofur-2-yl.pdf>

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