

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

Inchi:	InChI=1S/C7H4N4O5/c8-5(12)7-9-6(10-16-7)3-1-2-4(15-3)11(13)14/h1-2H,(H2,8,12)
InchiKey:	WQZXZPFIGQTAQE-UHFFFAOYSA-N
Formula:	C7H4N4O5
SMILES:	NC(=O)c1nc(-c2ccc([N+](=O)[O-])o2)no1
Mol. weight [g/mol]:	224.13
CAS:	36770-34-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.90		Crippen Method
logp	0.337		Crippen Method
mvol	131.240	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=C36770340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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