

Nifuratel

Inchi: InChI=1S/C10H11N3O5S/c1-19-6-8-5-12(10(14)18-8)11-4-7-2-3-9(17-7)13(15)16/h2-4,8
InchiKey: SRQKTCXJCCHINN-WCIBSUBMSA-N
Formula: C10H11N3O5S
SMILES: CSCC1CN(N=Cc2ccc([N+](=O)[O-])o2)C(=O)O1
Mol. weight [g/mol]: 285.28
CAS: 4936-47-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.89		Crippen Method
logp	1.706		Crippen Method
mcvol	184.180	ml/mol	McGowan Method
rinpol	2590.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C4936474&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/27-700-4/Nifuratel.pdf>

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