

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

Inchi: InChI=1S/C16H15N3O5/c1-2-3-10-22-12-6-4-11(5-7-12)16-17-15(18-24-16)13-8-9-14(23)
InchiKey: CVGDAZQIDRXOQF-UHFFFAOYSA-N
Formula: C16H15N3O5
SMILES: CCCCOC1CCC(-C2NC(-C3CC([N+](=O)[O-])O3)NO2)CC1
Mol. weight [g/mol]: 329.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.70		Crippen Method
logp	4.084		Crippen Method
mcvol	228.610	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009052&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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