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

Inchi: InChI=1S/C21H32BrN3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17(22)21-23-20(24-29-21)

InchiKey: CTUAECVBSGCAEU-UHFFFAOYSA-N

Formula: C21H32BrN3O4

SMILES: CCCCCCCCCCCCCCC(Br)c1nc(-c2ccc([N+](=O)[O-])o2)no1

Mol. weight [g/mol]: 470.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-18.86		Crippen Method
logp	7.765		Crippen Method
mcvol	334.450	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=B6009051&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume