

# 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:** CCCCCCCCCCCCCC(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/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](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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