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

Inchi: InChI=1S/C9H8BrN3O4/c1-2-5(10)9-11-8(12-17-9)6-3-4-7(16-6)13(14)15/h3-5H,2H2,1H3

InchiKey: CZQGCSVGEBXYOG-UHFFFAOYSA-N

Formula: C9H8BrN3O4

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

Mol. weight [g/mol]: 302.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.84		Crippen Method
logp	3.084		Crippen Method
mcvol	165.370	ml/mol	McGowan Method

Sources

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

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=B6009053&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume