Ribofuranose, 1-azido-1-deoxy-2,3-o-isopropylidene-, benzoate

Inchi: InChI=1S/C15H17N3O5/c1-15(2)22-11-10(21-13(17-18-16)12(11)23-15)8-20-14(19)9-6-4

InchiKey: MPHOYAKNKKOVOI-UHFFFAOYSA-N

Formula: C15H17N3O5

SMILES: CC1(C)OC2C(COC(=O)c3ccccc3)OC(N=[N+]=[N-])C2O1

Mol. weight [g/mol]: 319.31

CAS: 88237-98-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.33		Crippen Method
logp	2.399		Crippen Method
mcvol	223.120	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=C88237983&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