2-Furamidoxime, o-(3-pyridinecarbonyl)-5-nitro

Inchi: InChI=1S/C11H8N4O5/c12-10(8-3-4-9(19-8)15(17)18)14-20-11(16)7-2-1-5-13-6-7/h1-6H

InchiKey: FYMACIGRGPYGME-UHFFFAOYSA-N

Formula: C11H8N4O5

SMILES: NC(=NOC(=O)c1cccnc1)c1ccc([N+](=O)[O-])o1

Mol. weight [g/mol]: 276.20

CAS: 13353-88-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.66		Crippen Method
logp	1.060		Crippen Method
mcvol	179.000	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=C13353883&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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