2-Furoic acid, 5-nitro-, 1-phenylhydrazide

Inchi: InChI=1S/C11H9N3O4/c12-13(8-4-2-1-3-5-8)11(15)9-6-7-10(18-9)14(16)17/h1-7H,12H2
InchiKey: FDHAJEXURHGXFY-UHFFFAOYSA-N
Formula: C11H9N3O4
SMILES: NN(C(=O)c1ccc([N+](=O)[O-])o1)c1ccccc1
Mol. weight [g/mol]: 247.21
CAS: 103856-73-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.74		Crippen Method
logp	1.708		Crippen Method
mcvol	167.450	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=C103856731&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume