2-Furoic acid, 5-nitro-, 2-phenyl-1-hydrazide

Inchi: InChI=1S/C11H9N3O4/c15-11(9-6-7-10(18-9)14(16)17)13-12-8-4-2-1-3-5-8/h1-7,12H,(H,
InchiKey: CKMTVTCQCSEKSS-UHFFFAOYSA-N
Formula: C11H9N3O4
SMILES: O=C(NNc1ccccc1)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]: 247.21
CAS: 103854-67-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.01		Crippen Method
logp	1.945		Crippen Method
mcvol	167.450	ml/mol	McGowan Method

Sources

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=C103854677&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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