

2,4-dinitrophenylhydrazone furan-3-aldehyde

Inchi: InChI=1S/C11H8N4O5/c16-14(17)9-1-2-10(11(5-9)15(18)19)13-12-6-8-3-4-20-7-8/h1-7,10
InchiKey: VLLIRDRYDAQZQH-UHFFFAOYSA-N
Formula: C11H8N4O5
SMILES: O=[N+]([O-])c1ccc(NN=Cc2ccoc2)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 276.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.39		Crippen Method
logp	2.542		Crippen Method
mcvol	179.000	ml/mol	McGowan Method
rinpol	2657.00		NIST Webbook
rinpol	2657.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R139916&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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