

2-Furancarboxaldehyde, (2,4-dinitrophenyl)hydrazone

Inchi: InChI=1S/C11H8N4O5/c16-14(17)8-3-4-10(11(6-8)15(18)19)13-12-7-9-2-1-5-20-9/h1-7,10
InchiKey: JLMSXDMAAIAPCZ-UHFFFAOYSA-N
Formula: C11H8N4O5
SMILES: O=[N+](O-)c1ccc(NN=Cc2ccco2)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 276.20
CAS: 2074-02-4

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	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2074024&Units=SI>
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>

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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