2-Furoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C11H7NO5/c13-11(10-2-1-7-16-10)17-9-5-3-8(4-6-9)12(14)15/h1-7H
InchiKey: ATYBFDFZMSFCSW-UHFFFAOYSA-N
Formula: C11H7NO5
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1ccco1
Mol. weight [g/mol]: 233.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.94		Crippen Method
logp	2.407		Crippen Method
mcvol	153.360	ml/mol	McGowan Method
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook

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=U307998&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
rinpol: Non-polar retention indices

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