

Nicotinic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C12H8N2O4/c15-12(9-2-1-7-13-8-9)18-11-5-3-10(4-6-11)14(16)17/h1-8H
InchiKey: BRFXCDOSNZVQAQ-UHFFFAOYSA-N
Formula: C12H8N2O4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1cccnc1
Mol. weight [g/mol]: 244.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	2.209		Crippen Method
mcvol	167.260	ml/mol	McGowan Method
rinpol	2145.00		NIST Webbook
rinpol	2145.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307952&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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