

Nicotinic acid, 3-methylphenyl ester

Inchi: InChI=1S/C13H11NO2/c1-10-4-2-6-12(8-10)16-13(15)11-5-3-7-14-9-11/h2-9H,1H3
InchiKey: BUSZXQBIIPQKMP-UHFFFAOYSA-N
Formula: C13H11NO2
SMILES: Cc1cccc(OC(=O)c2cccnc2)c1
Mol. weight [g/mol]: 213.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	2.609		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
rinpole	1769.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307948&Units=SI>

Legend

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

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