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
rinpol	1769.00		NIST Webbook

Sources

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
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
rinpol:	Non-polar retention indices

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