

Nicotinic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C13H11NO3/c1-16-11-4-6-12(7-5-11)17-13(15)10-3-2-8-14-9-10/h2-9H,1H3
InchiKey: YKRYFWGYMGFVCO-UHFFFAOYSA-N
Formula: C13H11NO3
SMILES: COc1ccc(OC(=O)c2cccnc2)cc1
Mol. weight [g/mol]: 229.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	2.309		Crippen Method
mcvol	169.800	ml/mol	McGowan Method
rinsol	1935.00		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=U307949&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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