

Nicotinic acid, (4-methoxyphenyl)methyl ester

Inchi: InChI=1S/C14H13NO3/c1-17-13-6-4-11(5-7-13)10-18-14(16)12-3-2-8-15-9-12/h2-9H,10H
InchiKey: WMWSRFPILNHBNU-UHFFFAOYSA-N
Formula: C14H13NO3
SMILES: COc1ccc(COC(=O)c2cccnc2)cc1
Mol. weight [g/mol]: 243.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	2.447		Crippen Method
mcvol	183.890	ml/mol	McGowan Method
rinpole	2034.00		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=U308351&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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