

# Isonicotinic acid, (4-methoxyphenyl)methyl ester

**Inchi:** InChI=1S/C14H13NO3/c1-17-13-4-2-11(3-5-13)10-18-14(16)12-6-8-15-9-7-12/h2-9H,10H  
**InchiKey:** NRGHOBLIKFVENI-UHFFFAOYSA-N  
**Formula:** C14H13NO3  
**SMILES:** COc1ccc(COC(=O)c2ccncc2)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
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308347&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](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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