

# Nicotinic acid, 4-cyanophenyl ester

**Inchi:** InChI=1S/C13H8N2O2/c14-8-10-3-5-12(6-4-10)17-13(16)11-2-1-7-15-9-11/h1-7,9H  
**InchiKey:** UYGQOCITSPZWAZ-UHFFFAOYSA-N  
**Formula:** C13H8N2O2  
**SMILES:** N#Cc1ccc(OC(=O)c2cccnc2)cc1  
**Mol. weight [g/mol]:** 224.21

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.172		Crippen Method
mcvol	165.310	ml/mol	McGowan Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307950&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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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