

# Nicotinic acid, cyclobutyl ester

**Inchi:** InChI=1S/C10H11NO2/c12-10(13-9-4-1-5-9)8-3-2-6-11-7-8/h2-3,6-7,9H,1,4-5H2  
**InchiKey:** KFXYNZKFNAKUJG-UHFFFAOYSA-N  
**Formula:** C10H11NO2  
**SMILES:** O=C(OC1CCC1)c1cccnc1  
**Mol. weight [g/mol]:** 177.20

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	1.791		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
rinsol	1425.00		NIST Webbook
rinsol	1425.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299971&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  
**rinsol:** Non-polar retention indices

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