

# Nicotinic acid, morpholide

**Inchi:** InChI=1S/C10H12N2O2/c13-10(9-2-1-3-11-8-9)12-4-6-14-7-5-12/h1-3,8H,4-7H2  
**InchiKey:** QLPQPTXSAXQCMR-UHFFFAOYSA-N  
**Formula:** C10H12N2O2  
**SMILES:** O=C(c1ccnc1)N1CCOCC1  
**Mol. weight [g/mol]:** 192.21

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.20		Crippen Method
logp	0.554		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinsol	1706.00		NIST Webbook
rinsol	1706.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308103&Units=SI>

## 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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