

# Isonicotinic acid, 4-hexadecyl ester

**Inchi:** InChI=1S/C22H37NO2/c1-3-5-6-7-8-9-10-11-12-13-15-21(14-4-2)25-22(24)20-16-18-23-  
**InchiKey:** COYGRGBQNI AHMN-UHFFFAOYSA-N  
**Formula:** C22H37NO2  
**SMILES:** CCCCCCCCCCCC(CCC)OC(=O)c1ccncc1  
**Mol. weight [g/mol]:** 347.53

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.87		Crippen Method
logp	6.718		Crippen Method
mcvol	314.500	ml/mol	McGowan Method
rinpol	2458.00		NIST Webbook
rinpol	2458.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299969&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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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