

# Isonicotinic acid, 2-(1-adamantyl)ethyl ester

**Inchi:** InChI=1S/C18H23NO2/c20-17(16-1-4-19-5-2-16)21-6-3-18-10-13-7-14(11-18)9-15(8-13)  
**InchiKey:** VCUCWQUMMYGLLG-UHFFFAOYSA-N  
**Formula:** C18H23NO2  
**SMILES:** O=C(OCCC12CC3CC(CC(C3)C1)C2)c1ccncc1  
**Mol. weight [g/mol]:** 285.38  
**CAS:** 64140-42-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Crippen Method
logp	3.845		Crippen Method
mcvol	225.560	ml/mol	McGowan Method
rinpola	2328.00		NIST Webbook
rinpola	2328.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C64140427&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)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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