

# Isonicotinic acid, 1-adamantylmethyl ester

**Inchi:** InChI=1S/C17H21NO2/c19-16(15-1-3-18-4-2-15)20-11-17-8-12-5-13(9-17)7-14(6-12)10-  
**InchiKey:** DWZKGLSNCOFPKI-UHFFFAOYSA-N  
**Formula:** C17H21NO2  
**SMILES:** O=C(OCC12CC3CC(CC(C3)C1)C2)c1ccncc1  
**Mol. weight [g/mol]:** 271.35  
**CAS:** 64140-41-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	3.455		Crippen Method
mcvol	211.470	ml/mol	McGowan Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C64140416&Units=SI>

## 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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