

# Isonipecotic acid, N-acryloyl-, dodecyl ester

**Inchi:** InChI=1S/C21H37NO3/c1-3-5-6-7-8-9-10-11-12-13-18-25-21(24)19-14-16-22(17-15-19)2  
**InchiKey:** DSOXBYVGSYQBNS-UHFFFAOYSA-N  
**Formula:** C21H37NO3  
**SMILES:** C=CC(=O)N1CCC(C(=O)OCCCCCCCCCCCCC)CC1  
**Mol. weight [g/mol]:** 351.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	4.875		Crippen Method
mcvol	310.580	ml/mol	McGowan Method
rinpol	2806.00		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=U361061&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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