

# Isonipecotic acid, N-methacryloyl-, undecyl ester

Inchi:	InChI=1S/C21H37NO3/c1-4-5-6-7-8-9-10-11-12-17-25-21(24)19-13-15-22(16-14-19)20(2
InchiKey:	MFWPLFNOIOZXSU-UHFFFAOYSA-N
Formula:	C21H37NO3
SMILES:	C=C(C)C(=O)N1CCC(C(=O)OCCCCCCCCCCC)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
rmpol	2706.00		NIST Webbook
rmpol	2706.00		NIST Webbook

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360962&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360962&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

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

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