

Isonipecotic acid, N-allyloxycarbonyl-, heptyl ester

Inchi:	InChI=1S/C17H29NO4/c1-3-5-6-7-8-14-21-16(19)15-9-11-18(12-10-15)17(20)22-13-4-2/
InchiKey:	ZVPVUKDVBHPUGD-UHFFFAOYSA-N
Formula:	C17H29NO4
SMILES:	C=CCOC(=O)N1CCC(C(=O)OCCCCCCC)CC1
Mol. weight [g/mol]:	311.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	3.535		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
rinsol	2259.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinsol:	Non-polar retention indices

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