

Isonipecotic acid, N-allyloxycarbonyl-, propyl ester

Inchi: InChI=1S/C13H21NO4/c1-3-9-17-12(15)11-5-7-14(8-6-11)13(16)18-10-4-2/h4,11H,2-3,5
InchiKey: YHHUOYGAXFTJSY-UHFFFAOYSA-N
Formula: C13H21NO4
SMILES: C=CCOC(=O)N1CCC(C(=O)OCCC)CC1
Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.974		Crippen Method
mcvol	203.730	ml/mol	McGowan Method
rinpol	1861.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321988&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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
rinpol: Non-polar retention indices

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