

Isonipecotic acid, N-allyloxycarbonyl-, pentadecyl ester

Inchi:	InChI=1S/C25H45NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-22-29-24(27)23-17-19-26(2
InchiKey:	MUUHOEMAJQVJTJ-UHFFFAOYSA-N
Formula:	C25H45NO4
SMILES:	C=CCOC(=O)N1CCC(C(=O)OCCCCCCCCCCCCCCC)CC1
Mol. weight [g/mol]:	423.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.07		Crippen Method
logp	6.655		Crippen Method
mcvol	372.810	ml/mol	McGowan Method
rinpol	3274.00		NIST Webbook
rinpol	3274.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321999&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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