

Isonipecotic acid, N-allyloxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C24H43NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-21-28-23(26)22-16-18-25(19-1
InchiKey: STTBSTOIXLJRKC-UHFFFAOYSA-N
Formula: C24H43NO4
SMILES: C=CCOC(=O)N1CCC(C(=O)OCCCCCCCCCCCCCCC)CC1
Mol. weight [g/mol]: 409.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	6.265		Crippen Method
mcvol	358.720	ml/mol	McGowan Method
rinpola	3076.00		NIST Webbook
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Sources

Crippen Method: 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=U321998&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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