

Isonipecotic acid, N-allyloxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C16H27NO4/c1-4-11-21-16(19)17-9-7-14(8-10-17)15(18)20-12-5-6-13(2)3/h4,17-19,21
InchiKey: QAKNSRXOFKVFLI-UHFFFAOYSA-N
Formula: C₁₆H₂₇NO₄
SMILES: C=CCOC(=O)N1CCC(C(=O)OCCCC(C)C)CC1
Mol. weight [g/mol]: 297.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	3.000		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
rinpole	2113.00		NIST Webbook
rinpole	2113.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321992&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
rinpole: Non-polar retention indices

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