

Isonipecotic acid, N-allyloxycarbonyl-, hexyl ester

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	3.144		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321993&Units=SI>

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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