

Isonipecotic acid, N-(3-phenylpropionyl)-, decyl ester

Inchi: InChI=1S/C25H39NO3/c1-2-3-4-5-6-7-8-12-21-29-25(28)23-17-19-26(20-18-23)24(27)16
InchiKey: XIFAXECYWWWDPB-UHFFFAOYSA-N
Formula: C25H39NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)CCc2ccccc2)CC1
Mol. weight [g/mol]: 401.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.25		Crippen Method
logp	5.542		Crippen Method
mcvol	347.480	ml/mol	McGowan Method
rinpola	3326.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361563&Units=SI>
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>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/31-515-5/Isonipecotic-acid-N-3-phenylpropionyl-decyl-ester.pdf>

Generated by Cheméo on 2024-04-17 01:18:41.548648723 +0000 UTC m=+15605970.469226038.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.