

Isonipectic acid, N-(3-phenylpropionyl)-, nonyl ester

Inchi: InChI=1S/C24H37NO3/c1-2-3-4-5-6-7-11-20-28-24(27)22-16-18-25(19-17-22)23(26)15-1
InchiKey: CQFAPGRUPCFMAZ-UHFFFAOYSA-N
Formula: C24H37NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)CCc2ccccc2)CC1
Mol. weight [g/mol]: 387.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.83		Crippen Method
logp	5.152		Crippen Method
mcvol	333.390	ml/mol	McGowan Method
rinpol	3223.00		NIST Webbook
rinpol	3223.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361562&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

Latest version available from:

<https://www.cheméo.com/cid/27-009-2/Isonipectic-acid-N-3-phenylpropionyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-20 05:00:54.840626512 +0000 UTC m=+15878503.761203823.

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