

Isonipectic acid, N-(4-fluorobenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C27H42FNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-22-32-27(31)24-18-20-29(21-19)
InchiKey: HRMKKTQCBNUZFO-UHFFFAOYSA-N
Formula: C27H42FNO3
SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]: 447.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.00		Crippen Method
logp	6.922		Crippen Method
mcvol	377.430	ml/mol	McGowan Method
rinpol	3491.00		NIST Webbook
rinpol	3491.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361081&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/35-261-3/Isonipectic-acid-N-4-fluorobenzoyl-tetradecyl-ester.pdf>

Generated by Cheméo on 2024-04-20 05:16:32.183040755 +0000 UTC m=+15879441.103618071.

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