

L-Proline, N-(furoyl-2)-, tetradecyl ester

Inchi: InChI=1S/C24H39NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-29-24(27)21-16-14-18-25(21)
InchiKey: FPELQFMAVPOBLQ-UHFFFAOYSA-N
Formula: C24H39NO4
SMILES: CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc1
Mol. weight [g/mol]: 405.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.33		Crippen Method
logp	6.129		Crippen Method
mcvol	343.560	ml/mol	McGowan Method
rinpol	3134.00		NIST Webbook
rinpol	3134.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346115&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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<https://www.chemeo.com/cid/84-060-2/L-Proline-N-furoyl-2-tetradecyl-ester.pdf>

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