

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

Inchi: InChI=1S/C21H33NO4/c1-2-3-4-5-6-7-8-9-10-16-26-21(24)18-13-11-15-22(18)20(23)19-
InchiKey: WXOXICIVEZMSSL-UHFFFAOYSA-N
Formula: C21H33NO4
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc1
Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.08		Crippen Method
logp	4.958		Crippen Method
mcvol	301.290	ml/mol	McGowan Method
rinpol	2802.00		NIST Webbook
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Sources

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=U346113&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/84-635-4/L-Proline-N-furoyl-2-undecyl-ester.pdf>

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