

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

Inchi: InChI=1S/C19H29NO4/c1-2-3-4-5-6-7-8-14-24-19(22)16-11-9-13-20(16)18(21)17-12-10-
InchiKey: CQAUDJRJDYDOHJ-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc1
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.24		Crippen Method
logp	4.178		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
rinpol	2594.00		NIST Webbook
rinpol	2594.00		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=U346111&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

Latest version available from:

<https://www.chemeo.com/cid/96-390-3/L-Proline-N-furoyl-2-nonyl-ester.pdf>

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