

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

Inchi: InChI=1S/C28H47NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23-33-28(31)25-20-
InchiKey: BBQCOCCVKDGWJR-UHFFFAOYSA-N
Formula: C28H47NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccco1
Mol. weight [g/mol]: 461.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.01		Crippen Method
logp	7.689		Crippen Method
mcvol	399.920	ml/mol	McGowan Method
rinpol	3585.00		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=U346119&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/98-192-1/L-Proline-N-furoyl-2-octadecyl-ester.pdf>

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