

L-Proline, N-octanoyl-, nonyl ester

Inchi: InChI=1S/C22H41NO3/c1-3-5-7-9-10-12-14-19-26-22(25)20-16-15-18-23(20)21(24)17-18
InchiKey: LTBCHHKJIRQWOW-UHFFFAOYSA-N
Formula: C22H41NO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)CCCCCCC
Mol. weight [g/mol]: 367.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.25		Crippen Method
logp	5.632		Crippen Method
mcvol	328.970	ml/mol	McGowan Method
rinpol	2716.00		NIST Webbook
rinpol	2716.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U346244&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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