

L-Proline, N-(hexanoyl)-, nonyl ester

Inchi: InChI=1S/C20H37NO3/c1-3-5-7-8-9-10-12-17-24-20(23)18-14-13-16-21(18)19(22)15-11-12
InchiKey: XNZIBFVSEMULM-UHFFFAOYSA-N
Formula: C20H37NO3
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)CCCCC
Mol. weight [g/mol]: 339.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.41		Crippen Method
logp	4.851		Crippen Method
mcvol	300.790	ml/mol	McGowan Method
rinpol	2525.00		NIST Webbook
rinpol	2525.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346159&Units=SI>
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>

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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