

L-Proline, N-pivaloyl-, decyl ester

Inchi: InChI=1S/C20H37NO3/c1-5-6-7-8-9-10-11-12-16-24-18(22)17-14-13-15-21(17)19(23)20
InchiKey: NPRHMQVLRIWDFX-UHFFFAOYSA-N
Formula: C20H37NO3
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 339.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Crippen Method
logp	4.707		Crippen Method
mcvol	300.790	ml/mol	McGowan Method
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U346360&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/98-129-1/L-Proline-N-pivaloyl-decyl-ester.pdf>

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