L-Proline, N-pivaloyl-, undecyl ester

Inchi: InChI=1S/C21H39NO3/c1-5-6-7-8-9-10-11-12-13-17-25-19(23)18-15-14-16-22(18)20(24)21(2,3)4
InchiKey: APUZBAIHSOYBAO-UHFFFAOYSA-N
Formula: C21H39NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 353.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.59		Crippen Method
logp	5.097		Crippen Method
mcvol	314.880	ml/mol	McGowan Method
rinpol	2522.00		NIST Webbook
rinpol	2522.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346361&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.