L-Proline, N-pivaloyl-, tetradecyl ester

Inchi: InChI=1S/C24H45NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-20-28-22(26)21-18-17-19-25(
InchiKey: PNWXYRYVCKKFAO-UHFFFAOYSA-N
Formula: C24H45NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 395.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.84		Crippen Method
logp	6.268		Crippen Method
mcvol	357.150	ml/mol	McGowan Method
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook

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=U346362&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

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