L-Proline, N-pivaloyl-, hexadecyl ester

Inchi: InChI=1S/C26H49NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-30-24(28)23-20-19-
InchiKey: FQKHCORZSILBBK-UHFFFAOYSA-N
Formula: C26H49NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 423.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.68		Crippen Method
logp	7.048		Crippen Method
mcvol	385.330	ml/mol	McGowan Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		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=U346364&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

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