

L-Proline, N-pivaloyl-, octadecyl ester

Inchi: InChI=1S/C28H53NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-32-26(30)25-31
InchiKey: NQTZZGUIXVRRGO-UHFFFAOYSA-N
Formula: C28H53NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 451.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.52		Crippen Method
logp	7.828		Crippen Method
mcvol	413.510	ml/mol	McGowan Method
rinpol	3262.00		NIST Webbook
rinpol	3262.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346366&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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