L-Proline, N-octanoyl-, pentadecyl ester

Inchi: InChI=1S/C28H53NO3/c1-3-5-7-9-10-11-12-13-14-15-16-18-20-25-32-28(31)26-22-21-24
InchiKey: MMDUXOXPUJOBBL-UHFFFAOYSA-N
Formula: C28H53NO3
SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)CCCCCCC
Mol. weight [g/mol]: 451.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.76		Crippen Method
logp	7.972		Crippen Method
mcvol	413.510	ml/mol	McGowan Method
rinpol	3347.00		NIST Webbook
rinpol	3347.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346248&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

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