L-Proline, N-(octanoyl)-, isohexyl ester

Inchi: InChI=1S/C19H35NO3/c1-4-5-6-7-8-13-18(21)20-14-9-12-17(20)19(22)23-15-10-11-16(2
InchiKey: JFESWNUQCDCDMZ-UHFFFAOYSA-N
Formula: C19H35NO3
SMILES: CCCCCCCC(=O)N1CCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]: 325.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	4.317		Crippen Method
mcvol	286.700	ml/mol	McGowan Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		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=U346067&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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