

L-Proline, N-(3-methoxybenzoyl)-, isohexyl ester

Inchi: InChI=1S/C19H27NO4/c1-14(2)7-6-12-24-19(22)17-10-5-11-20(17)18(21)15-8-4-9-16(13)
InchiKey: HFSKGBIZKKGQAT-UHFFFAOYSA-N
Formula: C19H27NO4
SMILES: COc1cccc(C(=O)N2CCCC2C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	3.279		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		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=U346171&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.chemeo.com/cid/97-808-8/L-Proline-N-3-methoxybenzoyl-isohexyl-ester.pdf>

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