

Isonipecotic acid, N-(3-cyclopentylpropionyl)-, nonyl ester

Inchi: InChI=1S/C23H41NO3/c1-2-3-4-5-6-7-10-19-27-23(26)21-15-17-24(18-16-21)22(25)14-1
InchiKey: AGHBGYKNBBJXDT-UHFFFAOYSA-N
Formula: C23H41NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)CCC2CCCC2)CC1
Mol. weight [g/mol]: 379.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	5.489		Crippen Method
mcvol	332.200	ml/mol	McGowan Method
rinpol	3103.00		NIST Webbook
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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=U361089&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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