

Isonipecotic acid, N-(3-phenylpropionyl)-, pentyl ester

Inchi: InChI=1S/C20H29NO3/c1-2-3-7-16-24-20(23)18-12-14-21(15-13-18)19(22)11-10-17-8-5
InchiKey: VHXFMQJFHRUVSA-UHFFFAOYSA-N
Formula: C20H29NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)CCc2ccccc2)CC1
Mol. weight [g/mol]: 331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.591		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpol	2778.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361558&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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