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

Inchi: InChI=1S/C17H23NO3/c1-2-21-17(20)15-10-12-18(13-11-15)16(19)9-8-14-6-4-3-5-7-14/l

InchiKey: JJWKHNYMWXFXJG-UHFFFAOYSA-N

Formula: C17H23NO3

SMILES: CCOC(=O)C1CCN(C(=O)CCc2ccccc2)CC1

Mol. weight [g/mol]: 289.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.421		Crippen Method
mcvol	234.760	ml/mol	McGowan Method
rinpol	2466.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361554&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