

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/
InchiKey: JJWKHNYMWFJG-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
rinpola	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/ci9903071>
Crippen Method: https://www.cheméo.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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/48-206-0/Isonipecotic-acid-N-3-phenylpropionyl-ethyl-ester.pdf>

Generated by Cheméo on 2025-04-20 17:01:07.960725361 +0000 UTC m=+477513.461169599.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.