

Isonicotinic acid, 3-phenylpropyl ester

Inchi: InChI=1S/C15H15NO2/c17-15(14-8-10-16-11-9-14)18-12-4-7-13-5-2-1-3-6-13/h1-3,5-6,8
InchiKey: WSLXAZKWVHJXBO-UHFFFAOYSA-N
Formula: C15H15NO2
SMILES: O=C(OCCCCc1ccccc1)c1ccncc1
Mol. weight [g/mol]: 241.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.871		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308364&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

Latest version available from:

<https://www.chemeo.com/cid/93-515-7/Isonicotinic-acid-3-phenylpropyl-ester.pdf>

Generated by Cheméo on 2025-12-05 07:34:42.11029453 +0000 UTC m=+4668279.640335185.

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