

Isonicotinic acid, 2-phenylethyl ester

Inchi: InChI=1S/C14H13NO2/c16-14(13-6-9-15-10-7-13)17-11-8-12-4-2-1-3-5-12/h1-7,9-10H,8
InchiKey: TWVFPHQINDOCCO-UHFFFAOYSA-N
Formula: C14H13NO2
SMILES: O=C(OCCc1ccccc1)c1ccncc1
Mol. weight [g/mol]: 227.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	2.481		Crippen Method
mcvol	178.020	ml/mol	McGowan Method
rinpol	1839.00		NIST Webbook
rinpol	1839.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308363&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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