

Isonicotinic acid, phenylmethyl ester

Inchi: InChI=1S/C13H11NO2/c15-13(12-6-8-14-9-7-12)16-10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey: VXDBNGYOQMIPAT-UHFFFAOYSA-N
Formula: C13H11NO2
SMILES: O=C(OCc1ccccc1)c1ccncc1
Mol. weight [g/mol]: 213.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.439		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308346&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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