Nicotinic acid, 2-tetrahydrofurylmethyl ester

Inchi: InChI=1S/C11H13NO3/c13-11(9-3-1-5-12-7-9)15-8-10-4-2-6-14-10/h1,3,5,7,10H,2,4,6,8H
InchiKey: RQAITHJHUFFEIV-UHFFFAOYSA-N
Formula: C11H13NO3
SMILES: O=C(OCC1CCCO1)c1cccnc1
Mol. weight [g/mol]: 207.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	1.417		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308334&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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