Isonicotinamide, N-ethyl-N-(3-methylphenyl)-

Inchi: InChI=1S/C15H16N2O/c1-3-17(14-6-4-5-12(2)11-14)15(18)13-7-9-16-10-8-13/h4-11H,3H
InchiKey: XEAXCWYKTHEKCG-UHFFFAOYSA-N
Formula: C15H16N2O
SMILES: CCN(C(=O)c1ccncc1)c1cccc(C)c1
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	3.057		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
rinpol	1879.00		NIST Webbook
rinpol	1879.00		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=U308641&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.