Isonicotinamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C13H12N2O/c1-10-3-2-4-12(9-10)15-13(16)11-5-7-14-8-6-11/h2-9H,1H3,(H,15
InchiKey: OMZLQCLKNQSQQE-UHFFFAOYSA-N
Formula: C13H12N2O
SMILES: Cc1cccc(NC(=O)c2ccncc2)c1
Mol. weight [g/mol]: 212.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	2.642		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
rinpol	2042.00		NIST Webbook
rinpol	2042.00		NIST Webbook

Sources

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=U307413&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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