

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

Inchi: InChI=1S/C15H16N2O/c1-3-17(14-8-4-6-12(2)10-14)15(18)13-7-5-9-16-11-13/h4-11H,3H
InchiKey: VOUAHAXTCDDKHQ-UHFFFAOYSA-N
Formula: C15H16N2O
SMILES: CCN(C(=O)c1cccnc1)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	1936.00		NIST Webbook
rinpol	1936.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308471&Units=SI>
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>

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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<https://www.chemeo.com/cid/19-713-9/Nicotinamide-N-ethyl-N-3-methylphenyl.pdf>

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