

Nicotinamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C13H12N2O/c1-10-4-2-6-12(8-10)15-13(16)11-5-3-7-14-9-11/h2-9H,1H3,(H,15)
InchiKey: XZDOYZLZHKFSOX-UHFFFAOYSA-N
Formula: C13H12N2O
SMILES: Cc1cccc(NC(=O)c2cccnc2)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 |
| rinpola | 2065.00 | | 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=U308105&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/41-150-9/Nicotinamide-N-3-methylphenyl.pdf>

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