

2-Furancarboxamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C12H11NO2/c1-9-4-2-5-10(8-9)13-12(14)11-6-3-7-15-11/h2-8H,1H3,(H,13,14)
InchiKey: KPBVQSTXGSQMSM-UHFFFAOYSA-N
Formula: C12H11NO2
SMILES: Cc1cccc(NC(=O)c2ccco2)c1
Mol. weight [g/mol]: 201.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.66		Crippen Method
logp	2.840		Crippen Method
mcvol	154.140	ml/mol	McGowan Method
rinpol	1813.00		NIST Webbook
rinpol	1813.00		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=U307036&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

Latest version available from:

<https://www.chemeo.com/cid/22-937-7/2-Furancarboxamide-N-3-methylphenyl.pdf>

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