

2-Furancarboxamide, N-propyl-

Inchi: InChI=1S/C8H11NO2/c1-2-5-9-8(10)7-4-3-6-11-7/h3-4,6H,2,5H2,1H3,(H,9,10)
InchiKey: CGOIKKOEFBUPMP-UHFFFAOYSA-N
Formula: C8H11NO2
SMILES: CCCNC(=O)c1ccco1
Mol. weight [g/mol]: 153.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.39		Crippen Method
logp	1.419		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
rinsol	1358.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U407239&Units=SI>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/98-789-9/2-Furancarboxamide-N-propyl.pdf>

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