

2-Furancarboxamide, N-methyl-

Inchi: InChI=1S/C6H7NO2/c1-7-6(8)5-3-2-4-9-5/h2-4H,1H3,(H,7,8)
InchiKey: MXGRCIBAPXPYMA-UHFFFAOYSA-N
Formula: C6H7NO2
SMILES: CNC(=O)c1ccco1
Mol. weight [g/mol]: 125.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.55		Crippen Method
logp	0.639		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
rinsol	1230.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U407237&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.chemeo.com/cid/96-911-4/2-Furancarboxamide-N-methyl.pdf>

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