

2-Furancarboxamide, N-isobutyl-

Inchi: InChI=1S/C9H13NO2/c1-7(2)6-10-9(11)8-4-3-5-12-8/h3-5,7H,6H2,1-2H3,(H,10,11)
InchiKey: BYPSBNWZBFWJTR-UHFFFAOYSA-N
Formula: C9H13NO2
SMILES: CC(C)CNC(=O)c1ccco1
Mol. weight [g/mol]: 167.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.56		Crippen Method
logp	1.665		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
rinpole	1400.00		NIST Webbook
rinpole	1400.00		NIST Webbook

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=U407240&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/98-833-9/2-Furancarboxamide-N-isobutyl.pdf>

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