2-Furancarboxamide, N-butyl-

Inchi: InChI=1S/C9H13NO2/c1-2-3-6-10-9(11)8-5-4-7-12-8/h4-5,7H,2-3,6H2,1H3,(H,10,11)
InchiKey: VRJZWJSAYWGEJG-UHFFFAOYSA-N
Formula: C9H13NO2
SMILES: CCCCNC(=O)c1ccco1
Mol. weight [g/mol]: 167.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.81		Crippen Method
logp	1.809		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
rinpol	1461.00		NIST Webbook
rinpol	1461.00		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=U407241&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.