2-Furancarboxamide, N-heptyl-

Inchi: InChI=1S/C12H19NO2/c1-2-3-4-5-6-9-13-12(14)11-8-7-10-15-11/h7-8,10H,2-6,9H2,1H3,
InchiKey: UWWPDEMIIPFLRJ-UHFFFAOYSA-N
Formula: C12H19NO2
SMILES: CCCCCCCNC(=O)c1ccco1
Mol. weight [g/mol]: 209.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.06		Crippen Method
logp	2.980		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		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=U407247&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.