2-Furancarboxamide, N-(hept-2-yl)-

Inchi: InChI=1S/C12H19NO2/c1-3-4-5-7-10(2)13-12(14)11-8-6-9-15-11/h6,8-10H,3-5,7H2,1-2H
InchiKey: ANMUBJVQMXAPSJ-UHFFFAOYSA-N
Formula: C12H19NO2
SMILES: CCCCCC(C)NC(=O)c1ccco1
Mol. weight [g/mol]: 209.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.17		Crippen Method
logp	2.978		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		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=U407244&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

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