

2-Furancarboxamide, N-octyl-

Inchi: InChI=1S/C13H21NO2/c1-2-3-4-5-6-7-10-14-13(15)12-9-8-11-16-12/h8-9,11H,2-7,10H2,
InchiKey: FONXKBLTHHEHLU-UHFFFAOYSA-N
Formula: C13H21NO2
SMILES: CCCCCCCNC(=O)c1ccco1
Mol. weight [g/mol]: 223.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.48		Crippen Method
logp	3.370		Crippen Method
mcvol	191.990	ml/mol	McGowan Method
rinpole	1870.00		NIST Webbook
rinpole	1870.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407248&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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