

Sarcosine, N-(2-furoyl)-, hexyl ester

Inchi: InChI=1S/C14H21NO4/c1-3-4-5-6-9-19-13(16)11-15(2)14(17)12-8-7-10-18-12/h7-8,10H,
InchiKey: SRBJBEZGPYBXNN-UHFFFAOYSA-N
Formula: C14H21NO4
SMILES: CCCCCOC(=O)CN(C)C(=O)c1ccco1
Mol. weight [g/mol]: 267.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.14		Crippen Method
logp	2.475		Crippen Method
mcvol	213.520	ml/mol	McGowan Method
rinpola	2020.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321436&Units=SI>
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>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/64-579-9/Sarcosine-N-2-furoyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-19 21:01:26.871520715 +0000 UTC m=+15849735.792098032.

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