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: CCCCCCOC(=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
rinpol	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/ci990307l
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
rinpol: Non-polar retention indices