

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

Inchi: InChI=1S/C23H39NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-28-22(25)20-24(2)23(26)
InchiKey: LQBILBMKPRZTJY-UHFFFAOYSA-N
Formula: C23H39NO4
SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccco1
Mol. weight [g/mol]: 393.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.91		Crippen Method
logp	5.986		Crippen Method
mcvol	340.330	ml/mol	McGowan Method
rinpol	3045.00		NIST Webbook
rinpol	3045.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321444&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

Latest version available from:

<https://www.chemeo.com/cid/99-207-3/Sarcosine-N-2-furoyl-pentadecyl-ester.pdf>

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