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

Inchi: InChI=1S/C20H33NO4/c1-3-4-5-6-7-8-9-10-11-12-15-25-19(22)17-21(2)20(23)18-14-13-
InchiKey: XICWIVPLNSWUHS-UHFFFAOYSA-N
Formula: C20H33NO4
SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccco1
Mol. weight [g/mol]: 351.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.65		Crippen Method
logp	4.816		Crippen Method
mcvol	298.060	ml/mol	McGowan Method
rinpol	2645.00		NIST Webbook

Sources

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=U321442&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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