

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

Inchi:	InChI=1S/C26H45NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-31-25(28)23-27
InchiKey:	XYVKXYHAJRGXMI-UHFFFAOYSA-N
Formula:	C26H45NO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccco1
Mol. weight [g/mol]:	435.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.16		Crippen Method
logp	7.156		Crippen Method
mcvol	382.600	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321447&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

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<https://www.chemeo.com/cid/37-251-2/Sarcosine-N-2-furoyl-octadecyl-ester.pdf>

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