Isonipecotic acid, N-(2-furoyl)-, pentadecyl ester

Inchi: InChI=1S/C26H43NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-31-26(29)23-17-19-27(20-
InchiKey: VXEWXIMOXAIWST-UHFFFAOYSA-N
Formula: C26H43NO4
SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccco2)CC1
Mol. weight [g/mol]: 433.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.82		Crippen Method
logp	6.766		Crippen Method
mcvol	371.740	ml/mol	McGowan Method
rinpol	3465.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361512&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