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

Inchi: InChI=1S/C18H27NO4/c1-2-3-4-5-6-13-23-18(21)15-9-11-19(12-10-15)17(20)16-8-7-14-
InchiKey: QPUSYULQXBSYEJ-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCCCCCCOC(=O)C1CCN(C(=O)c2ccco2)CC1
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.47		Crippen Method
logp	3.645		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
rinpol	2606.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361505&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