

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

Inchi: InChI=1S/C20H31NO4/c1-2-3-4-5-6-7-8-15-25-20(23)17-11-13-21(14-12-17)19(22)18-10
InchiKey: FLIGZGPHHFSEOK-UHFFFAOYSA-N
Formula: C20H31NO4
SMILES: CCCCCCCCOC(=O)C1CCN(C(=O)c2ccco2)CC1
Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.31		Crippen Method
logp	4.426		Crippen Method
mcvol	287.200	ml/mol	McGowan Method
rinpol	2811.00		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=U361507&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

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