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

Inchi:	InChI=1S/C16H23NO4/c1-2-3-4-11-21-16(19)13-7-9-17(10-8-13)15(18)14-6-5-12-20-14/l
InchiKey:	NLHYMYYAKCKPGW-UHFFFAOYSA-N
Formula:	C16H23NO4
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2ccco2)CC1
Mol. weight [g/mol]:	293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	2.865		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
rinpol	2394.00		NIST Webbook
rinpol	2394.00		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=U361502&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

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