

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

Inchi:	InChI=1S/C17H25NO4/c1-2-3-4-5-12-22-17(20)14-8-10-18(11-9-14)16(19)15-7-6-13-21-
InchiKey:	VFFSRKHSLHPEIE-UHFFFAOYSA-N
Formula:	C17H25NO4
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2ccco2)CC1
Mol. weight [g/mol]:	307.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.05		Crippen Method
logp	3.255		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
rinpola	2504.00		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=U361504&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
rinpola:	Non-polar retention indices

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