

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

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.81		Crippen Method
logp	3.111		Crippen Method
mcpol	244.930	ml/mol	McGowan Method
rinpol	2462.00		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=U361503&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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