

Isonipecotic acid, N-(3-phenylpropionyl)-, octyl ester

Inchi:	InChI=1S/C23H35NO3/c1-2-3-4-5-6-10-19-27-23(26)21-15-17-24(18-16-21)22(25)14-13
InchiKey:	LQESBYHFNTUJNO-UHFFFAOYSA-N
Formula:	C23H35NO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)CCc2ccccc2)CC1
Mol. weight [g/mol]:	373.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.41		Crippen Method
logp	4.761		Crippen Method
mcvol	319.300	ml/mol	McGowan Method
rmpol	3117.00		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=U361561&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
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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