

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

Inchi:	InChI=1S/C21H31NO3/c1-2-3-4-8-17-25-21(24)19-13-15-22(16-14-19)20(23)12-11-18-9
InchiKey:	KQCOKBNSQGDGCF-UHFFFAOYSA-N
Formula:	C21H31NO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)CCc2ccccc2)CC1
Mol. weight [g/mol]:	345.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Crippen Method
logp	3.981		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
rinpola	2892.00		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=U361559&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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