

Isonipecotic acid, N-(cyclohexylcarbonyl)-, pentyl ester

Inchi:	InChI=1S/C18H31NO3/c1-2-3-7-14-22-18(21)16-10-12-19(13-11-16)17(20)15-8-5-4-6-9-
InchiKey:	HBZNBAXRUQATBW-UHFFFAOYSA-N
Formula:	C18H31NO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)C2CCCCC2)CC1
Mol. weight [g/mol]:	309.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	3.539		Crippen Method
mcvol	261.750	ml/mol	McGowan Method
rinpola	2536.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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