

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

Inchi:	InChI=1S/C20H35NO3/c1-2-3-4-7-16-24-20(23)18-12-14-21(15-13-18)19(22)11-10-17-8
InchiKey:	JUUSGGFGFAGZQG-UHFFFAOYSA-N
Formula:	C20H35NO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)CCC2CCCC2)CC1
Mol. weight [g/mol]:	337.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	4.319		Crippen Method
mcvol	289.930	ml/mol	McGowan Method
rinpola	2768.00		NIST Webbook
rinpola	2768.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361086&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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