

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

Inchi:	InChI=1S/C20H35NO3/c1-16(2)6-5-15-24-20(23)18-11-13-21(14-12-18)19(22)10-9-17-7
InchiKey:	FYIIETDBZSGRQD-UHFFFAOYSA-N
Formula:	C20H35NO3
SMILES:	CC(C)CCCOC(=O)C1CCN(C(=O)CCC2CCCC2)CC1
Mol. weight [g/mol]:	337.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	4.175		Crippen Method
mcvol	289.930	ml/mol	McGowan Method
rinpol	2728.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U361085&Units=SI

Legend

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

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