

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

Inchi:	InChI=1S/C26H47NO3/c1-2-3-4-5-6-7-8-9-10-13-22-30-26(29)24-18-20-27(21-19-24)25(
InchiKey:	SGKKASDCIUANLK-UHFFFAOYSA-N
Formula:	C26H47NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)CCC2CCCC2)CC1
Mol. weight [g/mol]:	421.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.22		Crippen Method
logp	6.659		Crippen Method
mcvol	374.470	ml/mol	McGowan Method
rinpol	3412.00		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=U361092&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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