

Isonipectic acid, N-(3-cyclopentylpropionyl)-, octyl ester

Inchi:	InChI=1S/C22H39NO3/c1-2-3-4-5-6-9-18-26-22(25)20-14-16-23(17-15-20)21(24)13-12-1
InchiKey:	MDZAEAVBSQDCTF-UHFFFAOYSA-N
Formula:	C22H39NO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)CCC2CCCC2)CC1
Mol. weight [g/mol]:	365.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.55		Crippen Method
logp	5.099		Crippen Method
mcvol	318.110	ml/mol	McGowan Method
rinsol	3000.00		NIST Webbook
rinsol	3000.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361088&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinsol:	Non-polar retention indices

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