

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

Inchi:	InChI=1S/C16H27NO3/c1-2-20-16(19)14-9-11-17(12-10-14)15(18)8-7-13-5-3-4-6-13/h13
InchiKey:	LHCQECNXCNROTF-UHFFFAOYSA-N
Formula:	C16H27NO3
SMILES:	CCOC(=O)C1CCN(C(=O)CCC2CCCC2)CC1
Mol. weight [g/mol]:	281.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	2.758		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
rinpola	2349.00		NIST Webbook
rinpola	2349.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U361083&Units=SI

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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