

Pipecolylpipecolic acid, N-ethoxycarbonyl-, dodecyl ester

Inchi:	InChI=1S/C27H48N2O5/c1-3-5-6-7-8-9-10-11-12-17-22-34-26(31)24-19-14-15-20-28(24)
InchiKey:	OMDXZYXGABCENJ-UHFFFAOYSA-N
Formula:	C27H48N2O5
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]:	480.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.76		Crippen Method
logp	5.843		Crippen Method
mcvol	405.980	ml/mol	McGowan Method
rinpol	3380.00		NIST Webbook
rinpol	3380.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393090&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
rinpol:	Non-polar retention indices

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