

Pipecolylpipecolic acid, N-propoxycarbonyl-, octyl ester

Inchi:	InChI=1S/C24H42N2O5/c1-3-5-6-7-8-13-19-30-23(28)21-15-10-11-16-25(21)22(27)20-14
InchiKey:	VMROSPDRWQNTIF-UHFFFAOYSA-N
Formula:	C24H42N2O5
SMILES:	CCCCCCCCOC(=O)C1CCCN1C(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]:	438.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	4.672		Crippen Method
mcvol	363.710	ml/mol	McGowan Method
rinpola	3033.00		NIST Webbook
rinpola	3033.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpola:	Non-polar retention indices

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