

# Pipecolic acid, N-propoxycarbonyl-, octadecyl ester

Inchi:	InChI=1S/C28H53NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-25-32-27(30)26-2
InchiKey:	MHUPTNMQTNLVMK-UHFFFAOYSA-N
Formula:	C28H53NO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C1CCCCN1C(=O)OCCC
Mol. weight [g/mol]:	467.72

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.82		Crippen Method
logp	8.192		Crippen Method
mcvol	419.380	ml/mol	McGowan Method
rinpola	3309.00		NIST Webbook
rinpola	3309.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393008&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393008&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## 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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