

# Pyrrolidine, 1-(1-oxooctadecyl)-

<b>Other names:</b>	Pyrrolidine, 1-stearoyl- 1-Stearoylpyrrolidine 1-Octadecanoylpyrrolidine
<b>Inchi:</b>	InChI=1S/C22H43NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22(24)23-20-17-18-2
<b>InchiKey:</b>	AEBDOCOLSSICMC-UHFFFAOYSA-N
<b>Formula:</b>	C22H43NO
<b>SMILES:</b>	CCCCCCCCCCCCCCCCC(=O)N1CCCC1
<b>Mol. weight [g/mol]:</b>	337.58
<b>CAS:</b>	33707-76-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.27		Crippen Method
logp	6.870		Crippen Method
mcvol	321.530	ml/mol	McGowan Method
rinsol	2742.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C33707765&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33707765&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307i">http://pubs.acs.org/doi/abs/10.1021/ci990307i</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinsol:</b>	Non-polar retention indices

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