

Pyrrolidine, 1-(1-oxo-2,5-octadecadienyl)-

Inchi:	InChI=1S/C22H39NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22(24)23-20-17-18-2
InchiKey:	QNBNFYKISNNUMZ-MHTUQYMHSA-N
Formula:	C22H39NO
SMILES:	CCCCCCCCCCCC=CCC=CC(=O)N1CCCC1
Mol. weight [g/mol]:	333.55
CAS:	56666-48-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.98		Crippen Method
logp	6.422		Crippen Method
mcvol	312.930	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56666489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/18-722-0/Pyrrolidine-1-1-oxo-2-5-octadecadienyl.pdf>

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