

# Furan-2-ylmethyl palmitate

**Inchi:** InChI=1S/C21H36O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-21(22)24-19-20-16-15-18-23  
**InchiKey:** SLLQRHYFOLOLLS-UHFFFAOYSA-N  
**Formula:** C21H36O3  
**SMILES:** CCCCCCCCCCCCCC(=O)OCc1ccco1  
**Mol. weight [g/mol]:** 336.51  
**CAS:** 95668-36-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-11.64		Crippen Method
logp	6.804		Crippen Method
mcvol	300.600	ml/mol	McGowan Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C95668363&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**rinpol:** Non-polar retention indices

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