

# Fentanyl, 4-N-(4-pentenyl) analogue

**Inchi:** InChI=1S/C19H28N2O/c1-3-5-9-14-20-15-12-18(13-16-20)21(19(22)4-2)17-10-7-6-8-11-  
**InchiKey:** CFTLBFPBPVNYCA-UHFFFAOYSA-N  
**Formula:** C19H28N2O  
**SMILES:** C=CCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1  
**Mol. weight [g/mol]:** 300.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	3.860		Crippen Method
mcvol	261.180	ml/mol	McGowan Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2364.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2367.00		NIST Webbook
rinpol	2346.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2356.00		NIST Webbook
rinpol	2346.00		NIST Webbook

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R637455&Units=SI>

# 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>rinpola:</b>	Non-polar retention indices

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