

# Fentanyl, 4-N-allyl analogue

**Inchi:** InChI=1S/C17H24N2O/c1-3-12-18-13-10-16(11-14-18)19(17(20)4-2)15-8-6-5-7-9-15/h3,5  
**InchiKey:** VDQNNKDVZMZHFLJ-UHFFFAOYSA-N  
**Formula:** C17H24N2O  
**SMILES:** C=CCN1CCC(N(C(=O)CC)c2ccccc2)CC1  
**Mol. weight [g/mol]:** 272.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	3.080		Crippen Method
mcvol	233.000	ml/mol	McGowan Method
rinpol	2196.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2186.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2186.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2193.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=R637480&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>rinpol:</b>	Non-polar retention indices

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