

# Para-fluorofentanyl

<b>Other names:</b>	p-Fluorofentanyl 4'-Fluoro fentanyl
<b>Inchi:</b>	InChI=1S/C22H27FN2O/c1-2-22(26)25(20-10-8-19(23)9-11-20)21-13-16-24(17-14-21)15
<b>InchiKey:</b>	KXUBAVLIJFTASZ-UHFFFAOYSA-N
<b>Formula:</b>	C22H27FN2O
<b>SMILES:</b>	CCC(=O)N(c1ccc(F)cc1)C1CCN(CCCc2ccccc2)CC1
<b>Mol. weight [g/mol]:</b>	354.46
<b>CAS:</b>	90736-23-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	4.276		Crippen Method
mcvol	285.760	ml/mol	McGowan Method
rinpol	2767.00		NIST Webbook
rinpol	2767.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C90736235&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C90736235&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/113-202-1/Para-fluorofentanyl.pdf>

Generated by Cheméo on 2024-04-23 12:04:52.959511414 +0000 UTC m=+16163141.880088742.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.