

# 4'-Chloro fentanyl

**Inchi:** InChI=1S/C22H27ClN2O/c1-2-22(26)25(20-10-8-19(23)9-11-20)21-13-16-24(17-14-21)1  
**InchiKey:** CUGMWAHBYRKBKL-UHFFFAOYSA-N  
**Formula:** C22H27ClN2O  
**SMILES:** CCC(=O)N(c1ccc(Cl)cc1)C1CCN(CCc2ccccc2)CC1  
**Mol. weight [g/mol]:** 370.92

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	4.790		Crippen Method
mcvol	296.230	ml/mol	McGowan Method
rinpole	2974.00		NIST Webbook
rinpole	2974.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R193089&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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