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)15
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
rinpol	2974.00		NIST Webbook
rinpol	2974.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R193089&Units=SI

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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