Para-fluorofentanyl

Other names:	p-Fluorofentanyl
	4'-Fluoro fentanyl
Inchi:	InChI=1S/C22H27FN2O/c1-2-22(26)25(20-10-8-19(23)9-11-20)21-13-16-24(17-14-21)15
InchiKey:	KXUBAVLIJFTASZ-UHFFFAOYSA-N
Formula:	C22H27FN2O
SMILES:	CCC(=O)N(c1ccc(F)cc1)C1CCN(CCc2ccccc2)CC1
Mol. weight [g/mol]:	354.46
CAS:	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90736235&Units=SI
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

Legend

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