Butanoyl 4'-fluoro fentanyl

Inchi:	InChI=1S/C24H31FN2O/c1-3-7-24(28)27(22-12-10-21(25)11-13-22)23-14-16-26(17-15-2
InchiKey:	RHAJTVXIFGHLMN-UHFFFAOYSA-N
Formula:	C24H31FN2O
SMILES:	CCCC(=O)N(c1ccc(F)cc1)C1CCN(C(C)Cc2ccccc2)CC1
Mol. weight [g/mol]:	382.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.98		Crippen Method
logp	5.054		Crippen Method
mcvol	313.940	ml/mol	McGowan Method
rinpol	2831.00		NIST Webbook
rinpol	2831.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R193183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:
https://www.chemeo.com/cid/77-383-2/Butanoyl-4-fluoro-fentanyl.pdf
Generated by Cheméo on 2024-04-29 09:51:54.315560391 +0000 UTC m=+16673563.236137706.

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