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

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=R193183&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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