N-Isobutanoyl 4'-fluoro fentanyl

Inchi: InChI=1S/C22H27FN2O/c1-17(2)22(26)25(20-10-8-19(23)9-11-20)21-12-14-24(15-13-21
InchiKey: XNQGKYHSTDKIKG-UHFFFAOYSA-N
Formula: C22H27FN2O
SMILES: CC(C)C(=O)N(c1ccc(F)cc1)C1CCN(Cc2ccccc2)CC1
Mol. weight [g/mol]: 354.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	4.479		Crippen Method
mcvol	285.760	ml/mol	McGowan Method
rinpol	2751.00		NIST Webbook
rinpol	2751.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R193252&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

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