Isobutanoyl 4'-chloro fentanyl

Inchi: InChI=1S/C24H31ClN2O/c1-18(2)24(28)27(22-11-9-21(25)10-12-22)23-13-15-26(16-14-2
InchiKey: ROSAEVLHZHLEKL-UHFFFAOYSA-N
Formula: C24H31ClN2O
SMILES: CC(C)C(=O)N(c1ccc(Cl)cc1)C1CCN(C(C)Cc2ccccc2)CC1
Mol. weight [g/mol]: 398.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.09		Crippen Method
logp	5.425		Crippen Method
mcvol	324.410	ml/mol	McGowan Method
rinpol	2955.00		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=R193207&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