Methyl-3-fentanyl

Other names: Butanoyl fentanyl
Inchi: InChI=1S/C23H30N2O/c1-2-9-23(26)25(21-12-7-4-8-13-21)22-15-18-24(19-16-22)17-14-
InchiKey: QQOMYEQLWQJRKK-UHFFFAOYSA-N
Formula: C23H30N2O
SMILES: CCCC(=O)N(c1ccccc1)C1CCN(CCc2ccccc2)CC1
Mol. weight [g/mol]: 350.50
CAS: 1169-70-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.11		Crippen Method
logp	4.527		Crippen Method
mcvol	298.080	ml/mol	McGowan Method
rinpol	2878.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1169706&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