Isobutanoyl fentanyl

Inchi: InChI=1S/C23H30N2O/c1-19(2)23(26)25(21-11-7-4-8-12-21)22-14-17-24(18-15-22)16-13
InchiKey: WRPFPNIHTOSMKU-UHFFFAOYSA-N
Formula: C23H30N2O
SMILES: CC(C)C(=O)N(c1ccccc1)C1CCN(CCc2ccccc2)CC1
Mol. weight [g/mol]: 350.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	4.383		Crippen Method
mcvol	298.080	ml/mol	McGowan Method
rinpol	2803.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R193212&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/99-224-4/Isobutanoyl-fentanyl.pdf
Generated by Cheméo on 2025-12-05 07:10:07.956903113 +0000 UTC m=+4666805.486943767.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.