«alpha»-Methyl butanoyl fentanyl

Inchi: InChI=1S/C24H32N2O/c1-3-10-24(27)26(22-13-8-5-9-14-22)23-15-17-25(18-16-23)20(2)
InchiKey: IPIGJTVNMCMXMT-UHFFFAOYSA-N
Formula: C24H32N2O
SMILES: CCCC(=O)N(c1ccccc1)C1CCN(C(C)Cc2ccccc2)CC1
Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	4.915		Crippen Method
mcvol	312.170	ml/mol	McGowan Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		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=R193158&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.