4''-Methoxy fentanyl

Inchi: InChI=1S/C23H30N2O2/c1-3-23(26)25(20-7-5-4-6-8-20)21-14-17-24(18-15-21)16-13-19-
InchiKey: LEUVPFMLRYUUGW-UHFFFAOYSA-N
Formula: C23H30N2O2
SMILES: CCC(=O)N(c1ccccc1)C1CCN(CCc2ccc(OC)cc2)CC1
Mol. weight [g/mol]: 366.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	4.145		Crippen Method
mcvol	303.950	ml/mol	McGowan Method
rinpol	3096.00		NIST Webbook
rinpol	3096.00		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=R193069&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.