Fentanyl, 4-N-nonyl analogue

Inchi: InChI=1S/C23H38N2O/c1-3-5-6-7-8-9-13-18-24-19-16-22(17-20-24)25(23(26)4-2)21-14-
InchiKey: ZWOWXODZUDOPQZ-UHFFFAOYSA-N
Formula: C23H38N2O
SMILES: CCCCCCCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]: 358.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	5.645		Crippen Method
mcvol	321.840	ml/mol	McGowan Method
rinpol	2765.00		NIST Webbook
rinpol	2780.00		NIST Webbook

Sources

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=R637544&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.