Fentanyl, 4-N-(5-hexenyl) analogue

Inchi: InChI=1S/C20H30N2O/c1-3-5-6-10-15-21-16-13-19(14-17-21)22(20(23)4-2)18-11-8-7-9-
InchiKey: FUTZNJGWIOVOHS-UHFFFAOYSA-N
Formula: C20H30N2O
SMILES: C=CCCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	4.250		Crippen Method
mcvol	275.270	ml/mol	McGowan Method
rinpol	2481.00		NIST Webbook
rinpol	2454.00		NIST Webbook
rinpol	2464.00		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=R637475&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