

Fentanyl, 4-N-hexyl analogue

Inchi: InChI=1S/C20H32N2O/c1-3-5-6-10-15-21-16-13-19(14-17-21)22(20(23)4-2)18-11-8-7-9-
InchiKey: VUCBDKQCPHDWDV-UHFFFAOYSA-N
Formula: C20H32N2O
SMILES: CCCCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	4.474		Crippen Method
mcvol	279.570	ml/mol	McGowan Method
rinpol	2450.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2474.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R637539&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

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