

N-Methyl butanoyl fentanyl

Inchi: InChI=1S/C16H24N2O/c1-3-7-16(19)18(14-8-5-4-6-9-14)15-10-12-17(2)13-11-15/h4-6,8-10,12-14,16-18,20-21/t16,18
InchiKey: GYCOYFSNPYCQOL-UHFFFAOYSA-N
Formula: C16H24N2O
SMILES: CCCC(=O)N(c1ccccc1)C1CCN(C)CC1
Mol. weight [g/mol]: 260.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.914		Crippen Method
mcvol	223.210	ml/mol	McGowan Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		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=R193272&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

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<https://www.chemeo.com/cid/115-989-7/N-Methyl-butanoyl-fentanyl.pdf>

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