N-Methyl acetyl fentanyl

Inchi: InChI=1S/C14H20N2O/c1-12(17)16(13-6-4-3-5-7-13)14-8-10-15(2)11-9-14/h3-7,14H,8-1
InchiKey: JRDQNWRUEQCCAW-UHFFFAOYSA-N
Formula: C14H20N2O
SMILES: CC(=O)N(c1ccccc1)C1CCN(C)CC1
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	2.134		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
rinpol	1952.00		NIST Webbook
rinpol	1952.00		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=R193267&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

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