

Acetamide, N-phenyl-N-[1-(1-phenyl-2-propyl)-4-piperidinyl]-

Other names:

«alpha»-Methyl acetyl fentanyl

«alpha»-Methylfentanyl acetyl analog

Inchi: InChI=1S/C22H28N2O/c1-18(20-9-5-3-6-10-20)17-23-15-13-22(14-16-23)24(19(2)25)21-

InchiKey: MDRBZPCJVBUXSG-UHFFFAOYSA-N

Formula: C22H28N2O

SMILES: CC(=O)N(c1ccccc1)C1CCN(CC(C)c2ccccc2)CC1

Mol. weight [g/mol]: 336.47

CAS: 90736-19-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	4.308		Crippen Method
mcvol	283.990	ml/mol	McGowan Method
rinpol	2819.00		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=C90736199&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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