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

Other names: Acetamide, N-phenyl-N-(1-benzyl-4-piperidinyl)-
N-Phenyl-N-(1-(phenylmethyl)-4-piperidinyl)acetamide
Piperidine, 1-benzyl-4-(N-phenylacetamido)-
N-Benzyl acetyl fentanyl

Inchi: InChI=1S/C20H24N2O/c1-17(23)22(19-10-6-3-7-11-19)20-12-14-21(15-13-20)16-18-8-4-

InchiKey: UKGXYSOSRSCGJB-UHFFFAOYSA-N

Formula: C20H24N2O

SMILES: CC(=O)N(c1ccccc1)C1CCN(Cc2ccccc2)CC1

Mol. weight [g/mol]: 308.42

CAS: 1237-52-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.704		Crippen Method
mcvol	255.810	ml/mol	McGowan Method
rinpol	2631.00		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=C1237521&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