«alpha»-Methylfentanyl

Other names: Propanamide, N-phenyl-N-[1-(1-phenylprop-2-yl)-4-piperidinyl]-
Inchi: InChI=1S/C23H30N2O/c1-3-23(26)25(21-12-8-5-9-13-21)22-14-16-24(17-15-22)19(2)18-
InchiKey: NGTVDHYUFBKWID-UHFFFAOYSA-N
Formula: C23H30N2O
SMILES: CCC(=O)N(c1ccccc1)C1CCN(C(C)Cc2ccccc2)CC1
Mol. weight [g/mol]: 350.50
CAS: 79704-88-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	4.525		Crippen Method
mcvol	298.080	ml/mol	McGowan Method
rinpol	2867.00		NIST Webbook
rinpol	2867.00		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=C79704884&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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