

3-Methylfentanyl

Other names:	Mefentanyl Propanamide, N-(3-methyl-1-(2-phenylethyl)-4-piperidiny)-N-phenyl- N-(3-Methyl-1-(2-phenylethyl)-4-piperidiny)-N-phenylpropanamide F 7209
Inchi:	InChI=1S/C23H30N2O/c1-3-23(26)25(21-12-8-5-9-13-21)22-15-17-24(18-19(22)2)16-14
InchiKey:	MLQRZXNZHAOCHQ-UHFFFAOYSA-N
Formula:	C23H30N2O
SMILES:	CCC(=O)N(c1ccccc1)C1CCN(CCc2ccccc2)CC1C
Mol. weight [g/mol]:	350.50
CAS:	42045-86-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	4.383		Crippen Method
mvol	298.080	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42045863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume

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