«alpha»-Methyl isobutanoyl fentanyl

Inchi:	InChI=1S/C24H32N2O/c1-19(2)24(27)26(22-12-8-5-9-13-22)23-14-16-25(17-15-23)20(3)
InchiKey:	UAMAVNLZTHVLCE-UHFFFAOYSA-N
Formula:	C24H32N2O
SMILES:	CC(C)C(=O)N(c1ccccc1)C1CCN(C(C)Cc2ccccc2)CC1
Mol. weight [g/mol]:	364.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	4.771		Crippen Method
mcvol	312.170	ml/mol	McGowan Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R193178&Units=SI

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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