

Fentanyl, 4-N-pentyl analogue

Inchi:	InChI=1S/C19H30N2O/c1-3-5-9-14-20-15-12-18(13-16-20)21(19(22)4-2)17-10-7-6-8-11-
InchiKey:	XBJSBLVYMJQONW-UHFFFAOYSA-N
Formula:	C19H30N2O
SMILES:	CCCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]:	302.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	4.084		Crippen Method
mcvol	265.480	ml/mol	McGowan Method

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=R637564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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