

Fentanyl, 4-N-octyl analogue

Inchi:	InChI=1S/C22H36N2O/c1-3-5-6-7-8-12-17-23-18-15-21(16-19-23)24(22(25)4-2)20-13-10
InchiKey:	CGZZCMMWVRVQCD-UHFFFAOYSA-N
Formula:	C22H36N2O
SMILES:	CCCCCCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]:	344.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.59		Crippen Method
logp	5.255		Crippen Method
mcvol	307.750	ml/mol	McGowan Method
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook
rinpol	2671.00		NIST Webbook
rinpol	2670.00		NIST Webbook
rinpol	2676.00		NIST Webbook
rinpol	2681.00		NIST Webbook
rinpol	2684.00		NIST Webbook
rinpol	2673.00		NIST Webbook
rinpol	2676.00		NIST Webbook
rinpol	2676.00		NIST Webbook
rinpol	2670.00		NIST Webbook
rinpol	2673.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R637559&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	https://link.springer.com/article/10.1007/BF02311772

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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