

Fentanyl, 4-N-propyl analogue

Inchi: InChI=1S/C17H26N2O/c1-3-12-18-13-10-16(11-14-18)19(17(20)4-2)15-8-6-5-7-9-15/h5-9
InchiKey: HDNAZKBGDIBSLJ-UHFFFAOYSA-N
Formula: C17H26N2O
SMILES: CCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]: 274.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	3.304		Crippen Method
mcvol	237.300	ml/mol	McGowan Method
rinpol	2166.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2187.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2185.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R637599&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
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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