Fentanyl, 4-N-propargyl analogue

Inchi: InChI=1S/C17H22N2O/c1-3-12-18-13-10-16(11-14-18)19(17(20)4-2)15-8-6-5-7-9-15/h1,5

InchiKey: FAGDRTQHLHVSLL-UHFFFAOYSA-N

Formula: C17H22N2O

SMILES: C#CCN1CCC(N(C(=O)CC)c2ccccc2)CC1

Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	2.527		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
rinpol	2218.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2232.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2231.00		NIST Webbook
rinpol	2232.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2239.00		NIST Webbook
rinpol	2218.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2239.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R637579&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices