Fentanyl, 4-N-(4-cyanobutyl) analogue

Inchi: InChI=1S/C19H27N3O/c1-2-19(23)22(17-9-5-3-6-10-17)18-11-15-21(16-12-18)14-8-4-7-
InchiKey: NTLIQBBVJIANCL-UHFFFAOYSA-N
Formula: C19H27N3O
SMILES: CCC(=O)N(c1ccccc1)C1CCN(CCCCC#N)CC1
Mol. weight [g/mol]: 313.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.588		Crippen Method
mcvol	266.860	ml/mol	McGowan Method
rinpol	2683.00		NIST Webbook
rinpol	2675.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2683.00		NIST Webbook
rinpol	2675.00		NIST Webbook
rinpol	2696.00		NIST Webbook
rinpol	2702.00		NIST Webbook
rinpol	2688.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2691.00		NIST Webbook
rinpol	2689.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R637440&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