Fentanyl, 4-N-(2-cyanoethyl) analogue

Inchi: InChI=1S/C17H23N3O/c1-2-17(21)20(15-7-4-3-5-8-15)16-9-13-19(14-10-16)12-6-11-18/
InchiKey: AMBTUOJRPJZOOM-UHFFFAOYSA-N
Formula: C17H23N3O
SMILES: CCC(=O)N(c1ccccc1)C1CCN(CCC#N)CC1
Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.808		Crippen Method
mcvol	238.680	ml/mol	McGowan Method
rinpol	2501.00		NIST Webbook
rinpol	2508.00		NIST Webbook
rinpol	2532.00		NIST Webbook
rinpol	2534.00		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2501.00		NIST Webbook
rinpol	2508.00		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2514.00		NIST Webbook

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=R637420&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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