Fentanyl, 4-N-(5-cyanopentyl) analogue

Inchi: InChI=1S/C20H29N3O/c1-2-20(24)23(18-10-6-5-7-11-18)19-12-16-22(17-13-19)15-9-4-3
InchiKey: LEZVNJYAKQHCLD-UHFFFAOYSA-N
Formula: C20H29N3O
SMILES: CCC(=O)N(c1ccccc1)C1CCN(CCCCCC#N)CC1
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	3.978		Crippen Method
mcvol	280.950	ml/mol	McGowan Method
rinpol	2786.00		NIST Webbook
rinpol	2742.00		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=R637460&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.