Fentanyl, 4-N-(3-butenyl) analogue

Inchi: InChI=1S/C18H26N2O/c1-3-5-13-19-14-11-17(12-15-19)20(18(21)4-2)16-9-7-6-8-10-16/l
InchiKey: KKAQHFNNAZOJDZ-UHFFFAOYSA-N
Formula: C18H26N2O
SMILES: C=CCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	3.470		Crippen Method
mcvol	247.090	ml/mol	McGowan Method

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=R637435&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