N-Benzyl butanoyl fentanyl

Inchi: InChI=1S/C22H28N2O/c1-2-9-22(25)24(20-12-7-4-8-13-20)21-14-16-23(17-15-21)18-19-
InchiKey: YYXPMGNUMFXSSW-UHFFFAOYSA-N
Formula: C22H28N2O
SMILES: CCCC(=O)N(c1ccccc1)C1CCN(Cc2ccccc2)CC1
Mol. weight [g/mol]: 336.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	4.484		Crippen Method
mcvol	283.990	ml/mol	McGowan Method
rinpol	2749.00		NIST Webbook
rinpol	2749.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R193232&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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

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