Fentanyl, 4-N-heptyl analogue

Inchi: InChI=1S/C21H34N2O/c1-3-5-6-7-11-16-22-17-14-20(15-18-22)23(21(24)4-2)19-12-9-8-
InchiKey: GKXBTMCVMRIGIY-UHFFFAOYSA-N
Formula: C21H34N2O
SMILES: CCCCCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]: 330.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Crippen Method
logp	4.864		Crippen Method
mcvol	293.660	ml/mol	McGowan Method
rinpol	2576.00		NIST Webbook
rinpol	2575.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2583.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2561.00		NIST Webbook
rinpol	2576.00		NIST Webbook
rinpol	2561.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2550.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R637524&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