Fentanyl, 4-N-undecyl analogue

Inchi: InChI=1S/C25H42N2O/c1-3-5-6-7-8-9-10-11-15-20-26-21-18-24(19-22-26)27(25(28)4-2)
InchiKey: BBKDDKZENHVNFZ-UHFFFAOYSA-N
Formula: C25H42N2O
SMILES: CCCCCCCCCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
Mol. weight [g/mol]: 386.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.85		Crippen Method
logp	6.425		Crippen Method
mcvol	350.020	ml/mol	McGowan Method
rinpol	2979.00		NIST Webbook
rinpol	2986.00		NIST Webbook
rinpol	2991.00		NIST Webbook
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
rinpol	2980.00		NIST Webbook
rinpol	2959.00		NIST Webbook
rinpol	2976.00		NIST Webbook
rinpol	2979.00		NIST Webbook
rinpol	2976.00		NIST Webbook
rinpol	2974.00		NIST Webbook
rinpol	2959.00		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=R637584&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