4-Anilino-N-Phenethylpiperidine

Other names:	Despropionyl fentanyl
	ANPP
	4-Piperidinamine, N-phenyl-1-(2-phenylethyl)-
	N-Phenyl-1-(2-phenylethyl)-4-piperidinamine
	4-anilino-N-phenethylpiperidine ("ANPP" or despropionylfentanyl) -
	4-Anilino-N-Phenethylpiperidine ("ANPP" or despropionylfentanyl) - from sample -
Inchi:	InChI=1S/C19H24N2/c1-3-7-17(8-4-1)11-14-21-15-12-19(13-16-21)20-18-9-5-2-6-10-18/
InchiKey:	ZCMDXDQUYIWEKB-UHFFFAOYSA-N
Formula:	C19H24N2
SMILES:	c1ccc(CCN2CCC(Nc3ccccc3)CC2)cc1
Mol. weight [g/mol]:	280.41
CAS:	21409-26-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.18		Crippen Method
logp	3.806		Crippen Method
mcvol	240.150	ml/mol	McGowan Method
rinpol	2529.80		NIST Webbook
rinpol	2529.80		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21409267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices