DESPROPIONYL FENTANYL

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

Physical Properties

Property code	Value	Unit	Source
hf	207.69	kJ/mol	Cheméo Relay (1.0)
hvap	111.59	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	Cheméo Relay (1.0)
logp	3.806		Crippen Method
mcvol	240.150	ml/mol	McGowan Method
rinpol	2529.80		NIST Webbook
rinpol	2529.80		NIST Webbook
tb	668.13	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21409267&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature