Valeryl fentanyl

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

1. GENERAL INFORMATION

IUPAC Name: *N*-phenyl- *N*-[1-(2-phenylethyl)piperidin-4-yl]pentanamide

CAS#: NA

Synonyms: Pentanoyl fentanyl; N-(1-phenethylpiperidin-4-yl)-N-phenylpentanamide

Source: DEA Reference Material Collection

Appearance: White Powder (HCl)

UV_{max}(nm): Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{24}H_{32}N_2O$	364	Not Determined
HCl	$C_{24}H_{32}N_2O$ HCl	400	Not Determined

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 mg/mL in CD_3OD containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}HNMR: Valeryl fentanyl HCl; Lot# RM-160223-01; CD_3OD; 400MHz

3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in $CHCl_3$

Instrument:	Agilent gas chromatograph operated in split mode with MS detector	
Column:	DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 µm	
Carrier Gas:	Helium at 0.9 mL/min	
Temperatures:	Injector: 280°C	MSD transfer line: 280°C
	MS Source: 230°C	MS Quad: 150°C
	Oven program:	
	1) 100°C initial temperature for 1.0 min	
	2) Ramp to 280°C at 12 °C/min	
	3) Hold final temperature for 9.0 min	
Injection Parameters:	Split Ratio = 25:1, 1 µL injected	
MS Parameters:	Mass scan range: 30-550 amu	Threshold: 150
	Tune file: stune.u	Acquisition mode: scan
Retention Time:	19.279 min	

EI Mass Spectrum: Valeryl fentanyl HCl; Lot# RM-160223-01

3.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm^{-1}
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): Valeryl fentanyl HCl; Lot# RM-160223-01

4. ADDITIONAL RESOURCES

No additional resources as of 06/2016