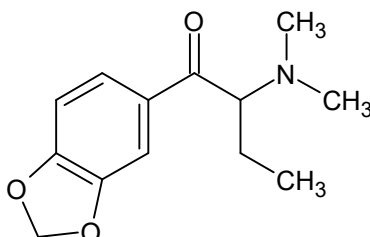




bk-DMBDB

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



1. GENERAL INFORMATION

IUPAC Name:	1-(2 <i>H</i> -1,3-benzodioxol-5-yl)-2-(dimethylamino)butan-1-one
CAS#:	802286-83-5 (base), 17763-12-1 (HCl)
Synonyms:	diButylone, Methylbutylone, B-ketone-N,N-dimethyl-1-(1,3-benzodioxol-5-yl)-2-butanamine
Source:	DEA Reference Material Collection
Appearance:	White Powder
UV_{max}(nm):	Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₃ H ₁₇ NO ₃	235	Not Determined
HCl	C ₁₃ H ₁₇ NO ₃ HCl	272	208.8



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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~6 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid 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

¹HNMR: bk-DMBDB HCl; Lot# 0432924-23; D₂O; 400MHz

