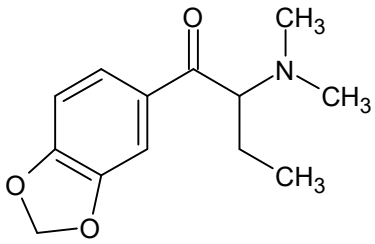
bk-DMBDB

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*H*-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 (^{0}C)
Base	$C_{13}H_{17}NO_3$	235	Not Determined
HCl	$C_{13}H_{17}NO_3$ HCl	272	208.8

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~6 mg/mL in D_2O 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

^{1}HNMR: bk-DMBDB HCl; Lot# 0432924-23: D_2O; 400MHz