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INGREDIENTS
TAJ GROUP

PRODUCT CODE- MTHDPHPRT177

Taj Pharmaceuticals Ltd.

3,4-METHYLENEDIOXYPHENYL-2-PROPANONE

741567 1211 MTH 758914

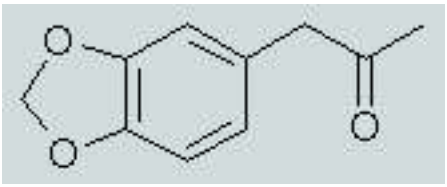
CAS No. 4676-39-5

IUPAC Name: 1-(1,3-benzodioxol-5-yl)propan-2-one

CAS Registry Number: 4676-39-5

Synonyms: Methyl piperonyl ketone, 5-Acetonyl-1,3-benzodioxole, 3,4-Methylenedioxyphenyl acetone, 3,4-Methylenedioxybenzyl methyl ketone, 1-(1,3-Benzodioxol-5-yl)acetone, CID78407, NSC16688, EINECS 225-128-6, 1-(Acetonyl)-3,4-methylenedioxybenzene, NSC 16688, ZINC01747237, (3,4-(Methylenedioxy)phenyl)-2-propanone, AI3-30059, 2-Propanone, 1-(1,3-benzodioxol-5-yl)-, 2-Propanone, (3,4-(methylenedioxy)phenyl)-, 2-Propanone, [3,4-(methylenedioxy)phenyl]-, 2-Propanone, 1-[3,4-(methylenedioxy)phenyl]-, 2-Propanone, 1-(1,3-benzodioxol-5-yl)- (9CI), 2-Propanone, 1-(3,4-(methylenedioxy)phenyl)- (8CI), 4676-39-5

Molecular Formula: C10H10O3 Molecular



Weight: 178.184600 [g/mol]

H-Bond Donor: 0 H-Bond Acceptor: 3

Chemical Name: PIPERONYL METHYL KETONE

3,4-methylenedioxy-phenyl-2-propanoneis a chemical compound consisting of phenylacetone substituted with a methylenedioxy functional group.

It is a chemical precursor of MDA, MDMA (more commonly known as "Ecstasy" or "XTC"), MDEA and related chemicalsMDP2P is most commonly synthesized by oxidizing the plant oil safrole or its isomer isosafrole using the Wacker oxidation or peroxyacid oxidation.

3,4-methylenedioxyphenyl)-2-propanone (MDP-2-P or PMK) was prepared by two different routes, i.e. by oxidizing isosafrole in an acid medium and by 1-(3,4-methylenedioxyphenyl)-2-nitropropene reduction.

The final product-MDP-2-P was subjected to GC/MS analysis.

The intermediates and reaction by-products were identified and the ‘route specific’ impurities were established.

3,4-methylenedioxyphenyl)butan-2-amine (MDP-2-MB, MBDB) is a new homologue of N-methyl-1-(3,4-methylenedioxyphenyl)propan-2-amine (MDMA), which is strictly controlled as a narcotic.
As part of our continuous survey on illegal designer drugs in the Japanese market, we found that N-methyl-4-(3,4-methylenedioxyphenyl)butan-2-amine (MDP-3-MB, HMDMA) was being sold as MBDB.

As this is the first time that HMDMA has been revealed to be in market distribution, and its physico-chemical data is thus far unreported, we describe the structure elucidation of HMDMA and comparative analysis with related compounds.
The impurity profiles were obtained by means of GC/MS, some reaction by-products were identified by means of the EI mass spectra including low energy EI mass spectra and 'route specific' impurities were established. 4-Methyl-5-(3,4-methylenedioxyphenyl)-[1,3]dioxolan-2-one ,N-methyl-2-methoxy-1-methyl-2-(3,4-methylenedioxyphenyl)-ethaneamine,3-methyl-6,7-methylenedioxyisoquinoline-1,4-dione and N-cyclohexyloacetamide were found to be the synthesis markers of greatest importance.

Abstract
This paper describes the structural elucidation of a compound produced during the synthesis of 3,4-methylenedioxymethylamphet-amine (MDMA) via the reductive amination of 3,4-methylenedioxyphenyl-2-propanone (3,4-MUP-2-P) with methylamine and sodium cyanoborohydride. The compound was isolated from MDMA by column chromatography, proton and carbon nuclear magnetic resonance spectroscopy, LC/mass spectrometry, and total synthesis were used to identify the compound as N-cyanomethyl-N-methyl-l-(3',4'-methylenedioxyphenyl)-2-propylamine.

This compound has been identified as a potential synthetic route marker for the reductive amination of 3,4-MDP-2-P with methylamine and sodium cyanoborohydride and as such it should prove valuable to forensic scientists engaged in profiling illicit drugs. Profiling MDMA can provide useful information to law enforcement agencies relating to synthetic route, precursor chemicals and reagents employed and may be used for comparative analyses of different drug seizures. This paper also describes the structural elucidation of the analogous methylamphetamine synthetic route marker compound, N-cyanomethyl-N-methyl-l-phenyl-2-propylamine, produced during the reductive amination of phenyl-2-propanone using methylamine and sodium cyanoborohydride.

Background
The investigation of clandestine drug manufacturing laboratories represents a combined effort between the criminal investigator and the forensic chemist. At an early point in an investigation the special agent will frequently request a list of the chemicals and synthesis methods used to produce a controlled substance. Providing these lists is often a very simple assignment the forensic chemist. A general understanding of various chemicals reactions and techniques is a part of the forensic chemist's training, academic background, and experience. Additionally, numerous specific and detailed drug syntheses are also available to him from the open literature. The chemist may, none the less, encounter problems when reviewing published procedures. If the literature procedures do not explicitly illustrate the synthesis of the desired pound, the chemist may erroneously assume that it is not applicable to the clandestine laboratory. This conclusion may, in part, be due to the complicated nature of the procedure or to the apparent requirement for specialized equipment. It may also arise from the failure of the chemist to visualize an application of the literature to the synthesis of the clandestine drug. In this context, the synthesis methods are themselves clandestine; they are "hidden" within the literature. A determined study of literature procedures, however, often reveals that while they do not detail the synthesis of the drug in question, they can be modified to give useful or simple methods for its manufacture. Sometimes this requires only the substitution of appropriate chemicals or certain changes in reaction parameters or catalysts.

Examples of this conceptual approach can be shown by the synthesis of the nonpsychoactive controlled substance phenyl-2-propanone (P-2-P). Halting the clandestine manufacture of P-2-P is of particular interest to enforcement personnel since it serves as the primary precursor in a number of syntheses for amphetamine and methamphetamine. By substitution of the chemicals and through slight changes in procedure, two published syntheses have been modified for P-2-P manufacture. These simple changes are illustrated below and are of the type to be expected of a clandestine drug chemist. By procuring chemicals and using procedures not generally recognized for the production of the controlled substance, the clandestine chemist may improve his chances to escape detection. Each of the two procedures investigated give fair to excellent yields of P-2-P, and, by using the procedures consecutively, yields are greatly increased.
Experimental

Procedure
The following procedure, which Tsuji et. al. [1] used for the preparation of 1-decanone, required only the substitution of allylbenzene (1-phenyl-2-propene) for 1- decene. A three-neck round bottomed flask was fitted with a magnetic stirrer and a pressure-equalized dropping funnel containing allylbenzene.

The flask was charged with a mixture of palladium chloride, cuprous chloride, and aqueous N,N-dimethylformamide (DMF). With all outlets securely stoppered and wired down, an oxygen-filled balloon was placed over one neck and the flask contents stirred at room temperature to allow oxygen uptake. After a period of oxygenation, allylbenzene was added dropwise. The solution was continuously stirred under the pressurized balloon. During this period of addition, the color of the solution turned from green to black and gradually returned to green as the reaction approached completion. The mixture was poured into cold hydrochloric acid and extracted with methylene chloride (CH2Cl2). The extract was washed with saturated sodium bicarbonate and dried over anhydrous sodium sulfate. Through filtration and distillation, phenyl-2-propanone and trans-beta-methylstyrene (1-phenyl-1-propene) were recovered.

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