

Synthesis of 5,5-diphenyl-3-(methylthiomethyl)hydantoin and 5,5-diphenyl-3-(methanesulfonylmethyl)hydantoin

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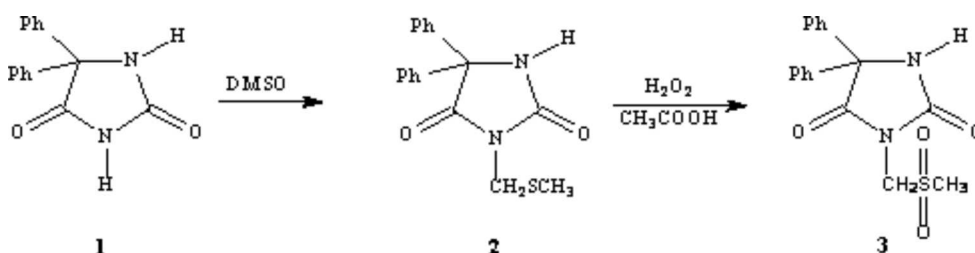
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Received: 9 October 2005 / Accepted: 18 October 2005 / Published: 31 March 2006

Keywords: hydantoin derivatives, DMSO, oxidation

In view of potential biological activity of 5,5-diphenylhydantoin derivatives (psychotropic agents)[1-3] we obtained 5,5-diphenyl-3-(methylthiomethyl)hydantoin (**2**) in reaction of 5,5-diphenylhydantoin (**1**) with DMSO and subsequently undergo its oxidation reaction to 5,5-diphenyl-3-(methanesulfonylmethyl)hydantoin (**3**) [4].



5,5-diphenyl-3-(methylthiomethyl)hydantoin (**2**)

A solution of 5,5-diphenylhydantoin (**1**) (commercial product) (17.5 g, 0.069 mol) in dimethylsulfoxide (DMSO, 350ml) was refluxed for 16 hrs, then cooled and poured into water (350 ml). The precipitated solid was filtered off, washed with water and dried. After two recrystallizations from methanol 5,5-diphenyl-3-methylthiomethylhydantoin (**2**, 20.5 g, 94.6%) was obtained as colorless needles.

Melting point: 124-131°C.

¹H NMR (DMSO-d₆, 80 MHz): δ= 9.80 (s, 1H, NH), 7.40 (s, 10H, Ph), 4.56 (s, 2H, CH₂), 2.15 (s, 3H, CH₃).

IR (KBr, cm⁻¹): 3270 (NH), 1780 (C=O).

MS (70eV) m/z (%): 312 (100), 297 (17.9), 265 (42.0), 251(67.9), 237 (100).

Elemental Analysis: Calculated for C₁₇H₁₆N₂O₂S (312.39): C 65.40, H 5.10, N 9.00; found C 65.20, H 5.10, N 8.80.

5,5-diphenyl-3-(methanesulfonylmethyl)hydantoin (**3**)

A solution of 5,5-diphenyl-3-(methylthiomethyl)hydantoin (**2**) (5.0 g, 0.016mol), glacial acetic acid (100 ml) and 30% H₂O₂ (100 ml) was allowed to stand at room temperature for 20 hrs. Then the solution was neutralized with 50% NaOH to pH 7. The precipitated solid was filtered off, washed several times with

water and dried. 5,5-Diphenyl-3-(methylsulfonyl-methyl)hydantoin (**3**, 5.1 g, 95.3%). After recrystallization from water-methanol (7:3) mixture, compound **3** as colorless needles (4.35 g, 81.3%) was obtained.

Melting point: 196-197°C

¹H NMR (DMSO-d₆, 80 MHz): δ= 9.98 (s, 1H, NH), 7.39 (s, 10H, Ph), 4.97 (s, 2H, CH₂), 3.15 (s, 3H, CH₃).

IR (KBr, cm⁻¹): 3365 (NH), 1785 and 1734 (C=O), 1140 (SO₂).

Elemental Analysis: Calculated for C₁₇H₁₆N₂O₄S (344.39): C 59.30, H 4.60, N 8.10; found C 59.10, H 4.60, N 8.00.

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Sample Availability: Available from MDPI.

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