

## Semicarbazone and Thiosemicarbazone of 5-acetyl-3-(methylsulfanyl)-1,2,4-triazine

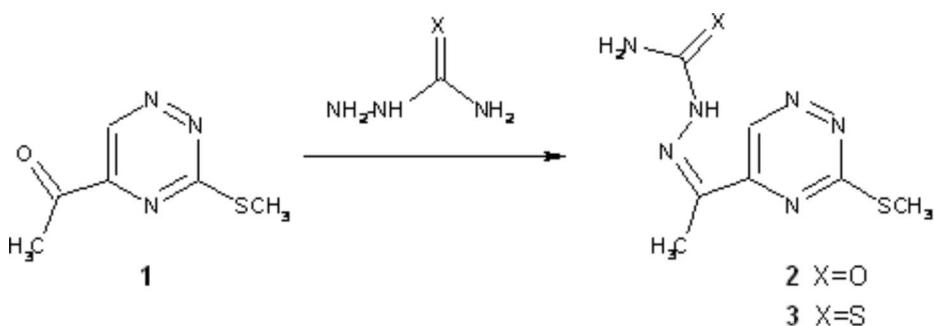
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Semicarbazone as well as thiosemicarbazone of 5-acetyl-3-(methylsulfanyl)-1,2,4-triazine were synthesised as reactive intermediates for the synthesis of 1*H*-pyrazolo[4,3-*e*][1,2,4]triazine derivatives *via* acid promoted ring closure [1-3].



Starting ketone **1** was prepared according to a reported procedure [4]. To a solution of ketone **1** (169 mg, 1 mmol) and semicarbazone or thiosemicarbazone (1.2 mmol) in ethanol (20 ml) 10% HCl (0.5 ml) was added. The resulting reaction mixture was heated at reflux for 5 min and then stirred at room temperature for additional 30 min. The precipitated solid was filtered off, recrystallized from dioxane and dried under vacuum.

### Semicarbazone of 5-acetyl-3-(methylsulfanyl)-1,2,4-triazine (**2**)

Yield 89%.

Melting Point: 260°C.

<sup>1</sup>H-NMR (200 MHz, DMSO-*d*<sub>6</sub>): δ= 2.19 (s, 3H); 2.62 (s, 3H); 6.96 (s, 2H, NH<sub>2</sub>); 9.98 (s, 1H); 10.13 (s, 1H, NH).

IR (CHCl<sub>3</sub> film, cm<sup>-1</sup>): 3339; 3106; 1693; 1520; 1486; 1426; 1312; 1256; 1183; 1133; 1058; 871; 713.

MS- EI (*m/z*, %): 226 (18) [M<sup>+</sup>]; 209 (7); 184 (11); 183 (100); 182 (62); 155 (12); 154 (39); 140 (32); 82 (49); 81 (30); 74 (18); 53 (19).

HR-MS: Calculated for C<sub>7</sub>H<sub>10</sub>N<sub>6</sub>OS: 226.0636. Found: 226.06314.

### Thiosemicarbazone of 5-acetyl-3-(methylsulfanyl)-1,2,4-triazine (**3**)

Yield 87%.

Melting Point: 229 °C.

IR (CHCl<sub>3</sub> film, cm<sup>-1</sup>): 3304; 3158; 2969; 1587; 1495; 1423; 1243; 1127; 1057; 876.

<sup>1</sup>H-NMR (200 MHz, DMSO-d<sub>6</sub>): δ= 2.31 (s, 3H); 2.63 (s, 3H); 8.53 (s, 1H); 8.70 (s, 1H); 10.08 (s, 1H); 10.81 (s, 1H).

MS-EI (*m/z*, %): 242 (80) [M<sup>+</sup>]; 199 (21); 167 (7); 154 (6); 141 (5); 140 (22); 128 (27); 116 (100); 82 (12); 81 (12); 74 (14); 60 (24); 53 (13).

HR-MS: Calculated for C<sub>7</sub>H<sub>10</sub>N<sub>6</sub>S<sub>2</sub>: 242.04084; Found: 242.04129.

#### References:

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*Sample Availability:* Available from MDPI.

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