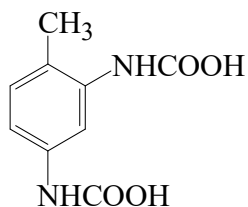




>>Entry Name: (4-Methyl-1,3-phenylene)biscarbamic acid, 9CI

Synonym(s): Toluene-2,4-dicarbamic acid, 8CI



**Molecular Formula:** C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>

**Molecular Weight:** 210.189

**Accurate Mass:** 210.064058

**Percentage Composition:** C 51.43%; H 4.80%; N 13.33%; O 30.45%

>>Derivative: Di-Me ester

Synonym(s): Obtucarbamate A

**CAS Registry Number:** 6935-99-5

**Molecular Formula:** C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>

**Molecular Weight:** 238.243

**Accurate Mass:** 238.095358

**Percentage Composition:** C 55.46%; H 5.92%; N 11.76%; O 26.86%

**Biological Source:** Constit. of the bark of *Chamaecyparis obtusa*

**Physical Description:** Cryst. (MeOH) or needles (Me<sub>2</sub>CO)

**Melting Point:** Mp 177° (168-169°)

>>Derivative: Di-Et ester

**CAS Registry Number:** 7450-62-6

**Molecular Formula:** C<sub>13</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>

**Molecular Weight:** 266.296

**Accurate Mass:** 266.126658

**Percentage Composition:** C 58.64%; H 6.81%; N 10.52%; O 24.03%

**Physical Description:** Cryst. (EtOH)

**Melting Point:** Mp 136°

>>Derivative: Dipropyl ester

**CAS Registry Number:** 60483-66-1

**Molecular Formula:** C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>

**Molecular Weight:** 294.35

**Accurate Mass:** 294.157958

**Percentage Composition:** C 61.21%; H 7.53%; N 9.52%; O 21.74%

**Physical Description:** Cryst. (petrol/EtOH)

**Melting Point:** Mp 109°

>>Derivative: Diisopropyl ester

**CAS Registry Number:** 42592-07-4

**Molecular Formula:** C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>

**Molecular Weight:** 294.35

**Accurate Mass:** 294.157958

**Percentage Composition:** C 61.21%; H 7.53%; N 9.52%; O 21.74%

**Physical Description:** Cryst.

**Melting Point:** Mp 136°

#### References:

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Panker, J.A. *et al.*, *J.O.C.*, 1957, **22**, 594-596, (*esters*)

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*Eur. Pat.*, 1981, 67 463; *CA*, **98**, 178994p, (*synth*)

Kuo, Y.H. *et al.*, *Chem. Express*, 1990, **5**, 909-912, (*Obtucarbamate A*)