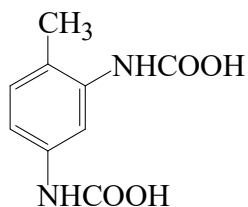




>>Entry Name: (4-Methyl-1,3-phenylene)biscarbamic acid, 9CI

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



Molecular Formula: C₉H₁₀N₂O₄

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: C₁₁H₁₄N₂O₄

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 (Me₂CO)

Melting Point: Mp 177° (168-169°)

>>Derivative: Di-Et ester

CAS Registry Number: 7450-62-6

Molecular Formula: C₁₃H₁₈N₂O₄

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: C₁₅H₂₂N₂O₄

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: C₁₅H₂₂N₂O₄

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:

Gaylord, N.G. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1955, **741**, 218-219, (*esters*)

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

Bossert, R.G. *et al.*, *J.O.C.*, 1958, **23**, 906-907, (*esters*)

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

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