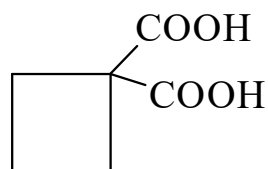




>>Entry Name: 1,1-Cyclobutanedicarboxylic acid, 9CI



CAS Registry Number: 5445-51-2

Molecular Formula: C<sub>6</sub>H<sub>8</sub>O<sub>4</sub>

Molecular Weight: 144.127

Accurate Mass: 144.04226

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Use/Importance: Has muscle relaxant and tranquillising props.

Physical Description: Prisms (H<sub>2</sub>O or Et<sub>2</sub>O)

Melting Point: Mp 157°

Solubility: Sol. H<sub>2</sub>O, Et<sub>2</sub>O, C<sub>6</sub>H<sub>6</sub>

pKa Value: pK<sub>a1</sub> 2.86; pK<sub>a2</sub> 5.22 (25°)

Aldrich: C9580-3

Fluka: 28680

>>Derivative: Di-Me ester

CAS Registry Number: 10224-72-3

Molecular Formula: C<sub>8</sub>H<sub>12</sub>O<sub>4</sub>

Molecular Weight: 172.18

Accurate Mass: 172.07356

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

Physical Description: Liq.

Boiling Point: Bp<sub>55</sub> 122°

>>Derivative: Di-Et ester

CAS Registry Number: 3779-29-1

Molecular Formula: C<sub>10</sub>H<sub>16</sub>O<sub>4</sub>

Molecular Weight: 200.234

Accurate Mass: 200.10486

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Physical Description: Liq.

Boiling Point: Bp 222-226°. Bp<sub>12</sub> 104°

Fluka: 28690

Rare Chemicals Library: S43617-8

>>Derivative: Diamide

CAS Registry Number: 33582-68-2

Molecular Formula: C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>

Molecular Weight: 142.157

Accurate Mass: 142.074228

Percentage Composition: C 50.69%; H 7.09%; N 19.71%; O 22.51%

Physical Description: Needles

Melting Point: Mp 275-277°

>>Derivative: *cis*-Diammineplatinum compd.

see Carboplatin, [BPB91-Q](#)

#### References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 840C, (*nmr*)  
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*Org. Synth.*, 1943, **23**, 16, (*synth*)  
*Org. Synth., Coll. Vol.*, 4, 1963, 288, (*ester*)  
Soltzberg, L. *et al.*, *J. Chem. Phys.*, 1971, **55**, 4907, (*cryst struct*)  
Dalton, L.R. *et al.*, *J.A.C.S.*, 1972, **94**, 6930, (*nmr*)  
Escalé, R. *et al.*, *Eur. J. Med. Chem. (Chim. Ther.)*, 1977, **12**, 501, (*synth*)  
Davis, C.R. *et al.*, *J.O.C.*, 1993, **58**, 6843, (*di-Me ester, synth, pmr, cmr, ms, ir*)