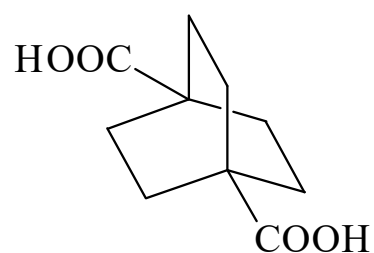




>>Entry Name: Bicyclo[2.2.2]octane-1,4-dicarboxylic acid



**CAS Registry Number:** 711-02-4

**Molecular Formula:** C<sub>10</sub>H<sub>14</sub>O<sub>4</sub>

**Molecular Weight:** 198.218

**Accurate Mass:** 198.08921

**Percentage Composition:** C 60.59%; H 7.12%; O 32.29%

**Melting Point:** Mp 360-370°

**pKa Value:** pK<sub>a1</sub> 4.47; pK<sub>a2</sub> 5.46 (25°)

>>Derivative: Mono-Me ester

**CAS Registry Number:** 18720-35-9

**Molecular Formula:** C<sub>11</sub>H<sub>16</sub>O<sub>4</sub>

**Molecular Weight:** 212.245

**Accurate Mass:** 212.10486

**Percentage Composition:** C 62.25%; H 7.60%; O 30.15%

**Physical Description:** Cryst. (C<sub>6</sub>H<sub>6</sub>)

**Melting Point:** Mp 180-182°

**pKa Value:** pK<sub>a1</sub> 4.76 (25°)

>>Derivative: Di-Me ester

**CAS Registry Number:** 1459-96-7

**Molecular Formula:** C<sub>12</sub>H<sub>18</sub>O<sub>4</sub>

**Molecular Weight:** 226.272

**Accurate Mass:** 226.12051

**Percentage Composition:** C 63.70%; H 8.02%; O 28.28%

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

**Melting Point:** Mp 98-100°

>>Derivative: Mono-Et ester

**CAS Registry Number:** 834-50-4

**Molecular Formula:** C<sub>12</sub>H<sub>18</sub>O<sub>4</sub>

**Molecular Weight:** 226.272

**Accurate Mass:** 226.12051

**Percentage Composition:** C 63.70%; H 8.02%; O 28.28%

**Physical Description:** Plates (C<sub>6</sub>H<sub>6</sub>/hexane)

**Melting Point:** Mp 149-150.5°

>>Derivative: Mono-Et ester amide

**Molecular Formula:** C<sub>12</sub>H<sub>19</sub>NO<sub>3</sub>

**Molecular Weight:** 225.287

**Accurate Mass:** 225.136494

**Percentage Composition:** C 63.98%; H 8.50%; N 6.22%; O 21.31%

**Physical Description:** Needles (C<sub>6</sub>H<sub>6</sub>/hexane)

**Melting Point:** Mp 143.6-145°

>>Derivative: Mono-Et ester nitrile

**Molecular Formula:** C<sub>12</sub>H<sub>17</sub>NO<sub>2</sub>

**Molecular Weight:** 207.272

**Accurate Mass:** 207.125929

**Percentage Composition:** C 69.54%; H 8.27%; N 6.76%; O 15.44%

**Boiling Point:** Bp<sub>5</sub> 146°. Bp<sub>0.7</sub> 115°

**References:**