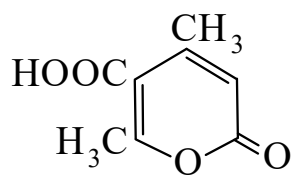




>>>Entry Name: 4,6-Dimethyl-2-oxo-2H-pyran-5-carboxylic acid, 9Cl

Synonym(s): Isodehydracetic acid. Isodehydroacetic acid



CAS Registry Number: 480-65-9

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

Molecular Weight: 168.149

Accurate Mass: 168.04226

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Physical Description: Needles or plates (H<sub>2</sub>O), prisms (EtOH)

Melting Point: Mp 155°

Solubility: Sol. hot H<sub>2</sub>O

pKa Value: pK<sub>a</sub> 2.28 (25°)

Other Data: Sublimes

Rare Chemicals Library: S94640-0

>>>Derivative: Me ester

CAS Registry Number: 41264-06-6

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

Molecular Weight: 182.176

Accurate Mass: 182.05791

Percentage Composition: C 59.34%; H 5.53%; O 35.13%

Physical Description: Needles (EtOH aq. or Et<sub>2</sub>O)

Melting Point: Mp 67-67.5°

Boiling Point: Bp<sub>30</sub> 188°

Aldrich: 19034-9

>>>Derivative: Et ester

CAS Registry Number: 3385-34-0

Molecular Formula: C<sub>10</sub>H<sub>12</sub>O<sub>4</sub>

Molecular Weight: 196.202

Accurate Mass: 196.07356

Percentage Composition: C 61.22%; H 6.16%; O 32.62%

Melting Point: Mp 17.5° (24.5°)

Boiling Point: Bp 285° dec.. Bp<sub>35</sub> 191°

Aldrich: E3340-8

Rare Chemicals Library: S70564-0

>>>Derivative: Anhydride

Physical Description: Cryst. (EtOH)

Melting Point: Mp 145-146°

>>>Derivative: Chloride

CAS Registry Number: 53891-40-0

Molecular Formula: C<sub>8</sub>H<sub>7</sub>ClO<sub>3</sub>

Molecular Weight: 186.594

Accurate Mass: 186.008372

Percentage Composition: C 51.50%; H 3.78%; Cl 19.00%; O 25.72%

Melting Point: Mp 52°

Boiling Point: Bp<sub>15</sub> 145-150°

#### References:

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*Org. Synth.*, *Coll. Vol.*, 4, 1963, 549, (*synth*)

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