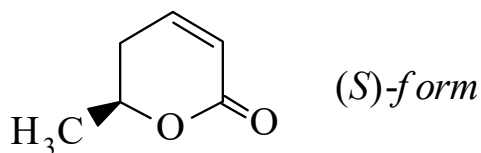




>>Entry Name: 5,6-Dihydro-6-methyl-2*H*-pyran-2-one, 9CI

Synonym(s): 2-Hexen-5-olide. Parasorbic acid



CAS Registry Number: 108-54-3

Molecular Formula: C₆H₈O₂

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Use/Importance: Bactericidal, antiprotozoal agent

Calculated Log P Data: Log P 0.41 (calc)

>>Variant: (*S*)-form

CAS Registry Number: 10048-32-5

Molecular Formula: C₆H₈O₂

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Biological Source: Constit. of rowan berries (*Sorbus aucuparia*)

Physical Description: Oil

Boiling Point: Bp₁₄ 104-105°

Optical Rotation: [α]_D²⁴ +206 (c, 1 in EtOH)

UV: [neutral] λ_{max} 205 (ε 10700) (MeOH) (Berdy) [neutral] λ_{max} 213 (ε 10000); 221 (ε 8100) (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, ipr) 250 mg/kg. Exp. neoplastic agent ; BERDY HAZD : LD₅₀ (mus, ipr) 250 mg/kg

>>Variant: (±)-form

CAS Registry Number: 10385-75-8

Molecular Formula: C₆H₈O₂

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Boiling Point: Bp₁₅ 110°. Bp_{0.05} 44°

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