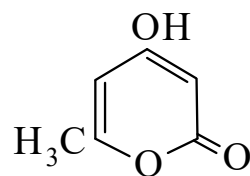




>>Entry Name: 4-Hydroxy-6-methyl-2H-pyran-2-one, 9CI

Synonym(s): Triacetic acid lactone



CAS Registry Number: 675-10-5

Molecular Formula: C₆H₆O₃

Molecular Weight: 126.112

Accurate Mass: 126.031695

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

Biological Source: Metab. of, *inter alia*, *Penicillium stipitatum*

Physical Description: Needles

Melting Point: Mp 190° (184-186°)

Other Data: Industrially available

Aldrich: H4341-5

Fluka: 55850

Rare Chemicals Library: S9648-3

>>Derivative: O-β-D-Glucopyranoside

CAS Registry Number: 221118-76-9

Molecular Formula: C₁₂H₁₆O₈

Molecular Weight: 288.254

Accurate Mass: 288.08452

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

Biological Source: Constit. of *Inulanthera nuda*

Physical Description: Amorph. powder

Optical Rotation: [α]_D −48 (c, 0.61 in H₂O)

UV: [neutral] λ_{max} 203 (log ε 3.88); 285 (log ε 3.3) (MeOH)

Other Data: Mp >185° dec.

>>Derivative: Ac

CAS Registry Number: 22073-80-9

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

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

Physical Description: Cryst. (toluene/hexane)

Melting Point: Mp 42-45°

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 31913-41-4

Molecular Formula: C₁₃H₁₂O₅S

Molecular Weight: 280.301

Accurate Mass: 280.040545

Percentage Composition: C 55.71%; H 4.31%; O 28.54%; S 11.44%

Physical Description: Pale yellow needles (EtOH)

Melting Point: Mp 102°