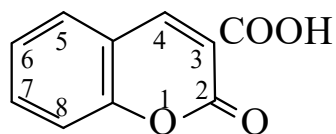




>>Entry Name: 2-Oxo-2H-1-benzopyran-3-carboxylic acid, 9CI

Synonym(s): Coumarin-3-carboxylic acid



CAS Registry Number: 531-81-7

Molecular Formula: C₁₀H₆O₄

Molecular Weight: 190.155

Accurate Mass: 190.02661

Percentage Composition: C 63.16%; H 3.18%; O 33.66%

Physical Description: Needles (H₂O)

Melting Point: Mp 187 dec.°

Other Data: Decarboxylates at 290°

Hazard & Toxicity: LD₅₀ (rat, orl) 200 mg/kg

Aldrich: C8560-3

Fluka: 28159

Rare Chemicals Library: S29191-9

>>Derivative: Me ester

CAS Registry Number: 21259-42-7

Molecular Formula: C₁₁H₈O₄

Molecular Weight: 204.182

Accurate Mass: 204.04226

Percentage Composition: C 64.71%; H 3.95%; O 31.34%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 116-117°

>>Derivative: Et ester

CAS Registry Number: 1846-76-0

Molecular Formula: C₁₂H₁₀O₄

Molecular Weight: 218.209

Accurate Mass: 218.05791

Percentage Composition: C 66.05%; H 4.62%; O 29.33%

Physical Description: Needles (EtOH)

Melting Point: Mp 94°

Aldrich: 39080-1

Rare Chemicals Library: S34820-1

>>Derivative: Amide

CAS Registry Number: 1846-78-2

Molecular Formula: C₁₀H₇NO₃

Molecular Weight: 189.17

Accurate Mass: 189.042594

Percentage Composition: C 63.49%; H 3.73%; N 7.40%; O 25.37%

Physical Description: Needles (AcOH)

Melting Point: Mp 268-269°. Mp 280-282°

>>Derivative: Anilide

CAS Registry Number: 54396-25-7

Molecular Formula: C₁₆H₁₁NO₃

Molecular Weight: 265.268

Accurate Mass: 265.073894

Percentage Composition: C 72.45%; H 4.18%; N 5.28%; O 18.09%

Physical Description: Yellow needles (EtOAc)

Melting Point: Mp 250°

Rare Chemicals Library: S14090-2