



>>Entry Name: **9*H*-Xanthene-9-carboxylic acid**, 9CI

Synonym(s): Xanthanoic acid

CAS Registry Number: 82-07-5

Molecular Formula: C₁₄H₁₀O₃

Molecular Weight: 226.231

Accurate Mass: 226.062995

Percentage Composition: C 74.33%; H 4.46%; O 21.22%

Use/Importance: Plant growth regulator. Has some antispasmodic activity

Melting Point: Mp 223-224°

Aldrich: X40-6

Fluka: 95480

>>Derivative: Me ester

CAS Registry Number: 39497-06-8

Molecular Formula: C₁₅H₁₂O₃

Molecular Weight: 240.258

Accurate Mass: 240.078645

Percentage Composition: C 74.99%; H 5.03%; O 19.98%

Melting Point: Mp 85-86°

>>Derivative: Et ester

CAS Registry Number: 7401-03-8

Molecular Formula: C₁₆H₁₄O₃

Molecular Weight: 254.285

Accurate Mass: 254.094295

Percentage Composition: C 75.58%; H 5.55%; O 18.88%

Melting Point: Mp 55-57°

>>Derivative: Chloride

Molecular Formula: C₁₄H₉ClO₂

Molecular Weight: 244.677

Accurate Mass: 244.029107

Percentage Composition: C 68.73%; H 3.71%; Cl 14.49%; O 13.08%

Physical Description: Needles (hexane)

Melting Point: Mp 87-88°

>>Derivative: Nitrile

Synonym(s): 9-Cyanoxanthene

CAS Registry Number: 85554-24-1

Molecular Formula: C₁₄H₉NO

Molecular Weight: 207.231

Accurate Mass: 207.068414

Percentage Composition: C 81.14%; H 4.38%; N 6.76%; O 7.72%

Physical Description: Needles (hexane)

Melting Point: Mp 99-100°

>>Derivative: Amide

CAS Registry Number: 5813-90-1

Molecular Formula: C₁₄H₁₁NO₂

Molecular Weight: 225.246

Accurate Mass: 225.078979

Percentage Composition: C 74.65%; H 4.92%; N 6.22%; O 14.21%

Physical Description: Cryst. (Py)

Melting Point: Mp 245-246°