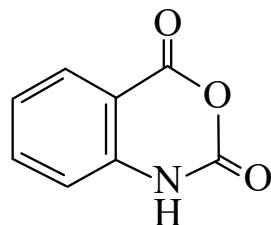




>>Entry Name: **2*H*-3,1-Benzoxazine-2,4(1*H*)-dione**, 9CI

Synonym(s): Isatoic anhydride



CAS Registry Number: 118-48-9

Molecular Formula: C₈H₅NO₃

Molecular Weight: 163.132

Accurate Mass: 163.026944

Percentage Composition: C 58.90%; H 3.09%; N 8.59%; O 29.42%

Physical Description: Cryst. (EtOH or dioxan)

Melting Point: Mp 243 dec.°

Hazard & Toxicity: Exp. reprod. effects

Aldrich: I-1280-8

Fluka: 58279

Sigma: I9131

>>Derivative: 1-Me

CAS Registry Number: 10328-92-4

Molecular Formula: C₉H₇NO₃

Molecular Weight: 177.159

Accurate Mass: 177.042594

Percentage Composition: C 61.02%; H 3.98%; N 7.91%; O 27.09%

Physical Description: Needles (CHCl₃/hexane)

Melting Point: Mp 165 dec.°

Aldrich: 12988-7

>>Derivative: 1-Et

CAS Registry Number: 50332-68-8

Molecular Formula: C₁₀H₉NO₃

Molecular Weight: 191.186

Accurate Mass: 191.058244

Percentage Composition: C 62.82%; H 4.74%; N 7.33%; O 25.11%

Physical Description: Cryst. (CH₂Cl₂)

Melting Point: Mp 121-123°

Rare Chemicals Library: S65702-6

>>Derivative: 1-Ph

CAS Registry Number: 20877-86-5

Molecular Formula: C₁₄H₉NO₃

Molecular Weight: 239.23

Accurate Mass: 239.058244

Percentage Composition: C 70.29%; H 3.79%; N 5.85%; O 20.06%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 177-179°

>>Derivative: 1-Benzyl

CAS Registry Number: 35710-05-5

Molecular Formula: C₁₅H₁₁NO₃

Molecular Weight: 253.257

Accurate Mass: 253.073894

Percentage Composition: C 71.14%; H 4.38%; N 5.53%; O 18.95%

Physical Description: Needles (C₆H₆/petrol)

Melting Point: Mp 140-141°

References: