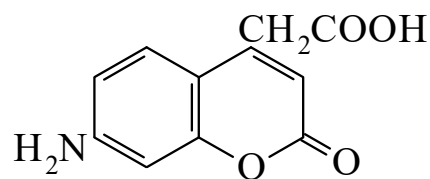




>>Entry Name: 7-Amino-2-oxo-2H-1-benzopyran-4-acetic acid, 9CI

Synonym(s): 7-Amino-4-coumarinacetic acid



CAS Registry Number: 85157-21-7

Molecular Formula: C₁₁H₉NO₄

Molecular Weight: 219.196

Accurate Mass: 219.053159

Percentage Composition: C 60.28%; H 4.14%; N 6.39%; O 29.20%

Physical Description: Pale yellow leaflets (EtOH)

Melting Point: Mp 224-225.5°. Mp 255° (dec.)

Other Data: The amine and its derivs. exhibit strong fluorescence in soln.

>>Derivative: Me ester

CAS Registry Number: 141692-65-1

Molecular Formula: C₁₂H₁₁NO₄

Molecular Weight: 233.223

Accurate Mass: 233.068809

Percentage Composition: C 61.80%; H 4.75%; N 6.01%; O 27.44%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 180°

>>Derivative: Et ester

CAS Registry Number: 95633-23-1

Molecular Formula: C₁₃H₁₃NO₄

Molecular Weight: 247.25

Accurate Mass: 247.084459

Percentage Composition: C 63.15%; H 5.30%; N 5.66%; O 25.88%

Physical Description: Orange needles (EtOH)

Melting Point: Mp 143-145 dec.°

>>Derivative: *N,N*-Di-Me

CAS Registry Number: 80883-54-1

Molecular Formula: C₁₃H₁₃NO₄

Molecular Weight: 247.25

Accurate Mass: 247.084459

Percentage Composition: C 63.15%; H 5.30%; N 5.66%; O 25.88%

Use/Importance: Fluorescent probe

Physical Description: Yellow needles (EtOH aq.)

Melting Point: Mp 185 dec.° (168° dec.)

References:

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Tolmachev, A.I. *et al.*, *Zh. Obshch. Khim.*, 1963, **33**, 440; *J. Gen. Chem. USSR (Engl. Transl.)*, 1963, **33**, 433, (*N,N*-di-Me)

Kanaoka, Y. *et al.*, *Chem. Pharm. Bull.*, 1984, **32**, 3926, (*synth*, *ir*, *pmr*)

Besson, T. *et al.*, *Heterocycles*, 1992, **34**, 273, (*synth*, *uv*, *ir*, *pmr*)

Charitos, C. *et al.*, *J. Het. Chem.*, 2001, **38**, 153-158, (*synth*, *pmr*)