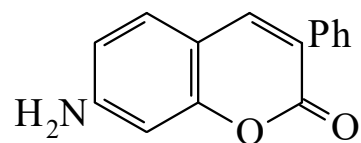




>>Entry Name: 7-Amino-3-phenyl-2H-1-benzopyran-2-one

Synonym(s): 7-Amino-3-phenylcoumarin, 8Cl



CAS Registry Number: 4108-61-6

Molecular Formula: C₁₅H₁₁NO₂

Molecular Weight: 237.257

Accurate Mass: 237.078979

Percentage Composition: C 75.94%; H 4.67%; N 5.90%; O 13.49%

Physical Description: Yellow needles

Melting Point: Mp 208-209°

>>Derivative: N-Ac

Molecular Formula: C₁₇H₁₃NO₃

Molecular Weight: 279.295

Accurate Mass: 279.089544

Percentage Composition: C 73.11%; H 4.69%; N 5.02%; O 17.19%

Physical Description: Needles (methycellosolve)

Melting Point: Mp 265°

>>Derivative: N-(4-Methylbenzenesulfonyl)

CAS Registry Number: 103825-73-6

Molecular Formula: C₂₂H₁₇NO₄S

Molecular Weight: 391.447

Accurate Mass: 391.087829

Percentage Composition: C 67.50%; H 4.38%; N 3.58%; O 16.35%; S 8.19%

Physical Description: Needles (EtOH)

Melting Point: Mp 241°

References:

U.S. Pat., 1960, 2 929 822; CA, **55**, 4538c, (synth, Ac)

U.S. Pat., 1970, 3 514 471; CA, **73**, 35221g, (synth)

Shibryaeva, L.S. et al., Zh. Obshch. Khim., 1980, **50**, 940; J. Gen. Chem. USSR (Engl. Transl.), 1980, **50**, 763, (ms)

Honda, T. et al., Acta Cryst. C, 1996, **52**, 899, (cryst struct)