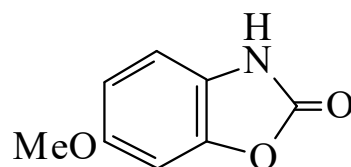




>>Entry Name: 6-Methoxy-2(3*H*)-benzoxazolone, 9CI

ENTRY UNDER REVIEW

Synonym(s): 6-Methoxy-2-benzoxazolinone, 8CI. Coixol. MBOA



CAS Registry Number: 532-91-2

Molecular Formula: C₈H₇NO₃

Molecular Weight: 165.148

Accurate Mass: 165.042594

Percentage Composition: C 58.18%; H 4.27%; N 8.48%; O 29.06%

Secale cereale). Also present in all plant parts of *Scoparia dulcis* (Scrophulariaceae)

Use/Importance: Disease and insect attack inhibitor

Physical Description: Pink cryst. (MeOH aq.)

Melting Point: Mp 160-161° (154-155°)

Solubility: BERDY SOL: Sol. bases, EtOH, Et₂O, C₆H₆; fairly sol. H₂O; poorly sol. hexane

UV: [neutral] λ_{max} 229 (); 286 () (H₂O) (Berdy)

Sigma: M0640

>>Derivative: *N*-Ac

CAS Registry Number: 62655-08-7

Molecular Formula: C₁₀H₉NO₄

Molecular Weight: 207.185

Accurate Mass: 207.053159

Percentage Composition: C 57.97%; H 4.38%; N 6.76%; O 30.89%

Physical Description: Needles

Melting Point: Mp 147.5°

>>Derivative: *N*-Benzoyl

Molecular Formula: C₁₅H₁₁NO₄

Molecular Weight: 269.256

Accurate Mass: 269.068809

Percentage Composition: C 66.91%; H 4.12%; N 5.20%; O 23.77%

Physical Description: Needles

Melting Point: Mp 162-162.5°

>>Derivative: 5-Chloro

Synonym(s): 5-Chloro-6-methoxy-2(3*H*)-benzoxazolone. 5-Chloro-6-methoxy-2-benzoxazolinone

Molecular Formula: C₈H₆ClNO₃

Molecular Weight: 199.593

Accurate Mass: 199.003621

Percentage Composition: C 48.14%; H 3.03%; Cl 17.76%; N 7.02%; O 24.05%

Biological Source: Isol. from *Zea mays*

References:

- Koyama, T. *et al.*, *Yakugaku Zasshi*, 1955, **75**, 699
Virtanen, A.I. *et al.*, *Suom. Kemistil. B*, 1956, **29**, 143; 171
List, P.H., *Arch. Pharm. (Weinheim, Ger.)*, 1959, **292**, 452
Allen, E.H. *et al.*, *J.O.C.*, 1971, **36**, 2004, (*synth*)
Richey, J.D. *et al.*, *Agric. Biol. Chem.*, 1976, **40**, 2413, (*synth*)
Kubo, I. *et al.*, *Experientia*, 1983, **39**, 355, (*isol, synth*)
Sicher, D., *Synthesis*, 1989, 875, (*synth*)
Maleski, R.J. *et al.*, *J. Het. Chem.*, 1991, **28**, 1937, (*synth*)
Bjostad, L.B. *et al.*, *J. Chem. Ecol.*, 1992, **18**, 931
Hayashi, T. *et al.*, *Phytochemistry*, 1994, **37**, 1611, (*isol, occur*)
Kato-Noguchi, H. *et al.*, *Phytochemistry*, 1998, **49**, 433-435, (*5-chloro*)