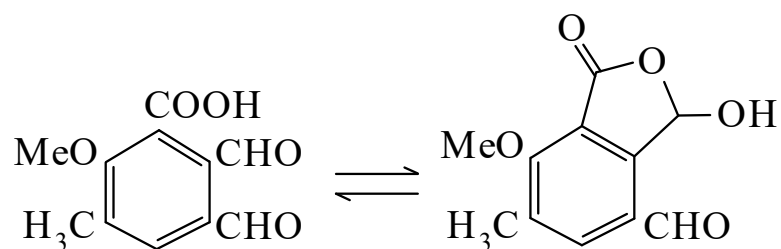




>>Entry Name: **2,3-Diformyl-6-methoxy-5-methylbenzoic acid**, 9CI

Synonym(s): 5,6-Diformyl-2-methoxy-*m*-toluic acid. **Gladiolic acid**



CAS Registry Number: 478-05-7

Molecular Formula: C₁₁H₁₀O₅

Molecular Weight: 222.197

Accurate Mass: 222.052825

Percentage Composition: C 59.46%; H 4.54%; O 36.00%

Biological Source: Metab. of *Penicillium gladioli*

Use/Importance: Antifungal antibiotic

Physical Description: Silky needles (H₂O)

Melting Point: Mp 160°

Solubility: Sol. hot H₂O, Me₂CO, EtOH, AcOH; BERDY SOL: Sol. MeOH, dioxan, AcOH, Me₂CO, bases, CHCl₃; fairly sol. H₂O, Et₂O; poorly sol. C₆H₆, CCl₄, hexane

pKa Value: pK_a 4.4 (H₂O)

UV: [neutral] λ_{max} 214 (ε 18500); 271 (ε 6900); 304 (ε 3200) (MeOH) (Berdy) [acid] λ_{max} 269 (ε 10960); 306 (ε 4470) (pH 4 buffer) (Berdy) [base] λ_{max} 275 (ε 3390); 343 (ε 660) (NAOH) (Berdy)

>>Derivative: Hemihydrate

Physical Description: Prisms

Melting Point: Mp 155°

>>Derivative: Na salt

Physical Description: Needles + 2 or 3H₂O

Melting Point: Mp 230 dec.°

Other Data: Trihydrate loses 1H₂O at 180°

>>Derivative: Me ester

Molecular Formula: C₁₂H₁₂O₅

Molecular Weight: 236.224

Accurate Mass: 236.068475

Percentage Composition: C 61.02%; H 5.12%; O 33.86%

Physical Description: Needles (MeOH)

Melting Point: Mp 140°

Solubility: Insol. H₂O

>>Derivative: Me ester, 2,4-dinitrophenylhydrazone

Melting Point: Mp 245-250 dec.°

>>Derivative: Et ester

Molecular Formula: C₁₃H₁₄O₅

Molecular Weight: 250.251

Accurate Mass: 250.084125

Percentage Composition: C 62.39%; H 5.64%; O 31.97%

Physical Description: Needles (EtOH)

Melting Point: Mp 105°

References:

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Grove, B., *Biochem. J.*, 1952, **50**, 648, (*isol, struct*)

Grove, J.F., *J.C.S.*, 1952, 3345, (*ir*)

Brown, P. *et al.*, *Chem. Ind. (London)*, 1953, 1151, (*struct*)

Brown, J.J. *et al.*, *J.C.S.*, 1954, 1076, (*synth*)