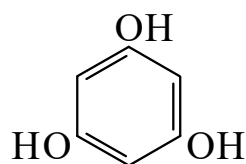




>>Entry Name: **1,3,5-Benzenetriol**, 9CI

ENTRY UNDER REVIEW

Synonym(s): 1,3,5-Trihydroxybenzene. **Phloroglucinol**. Phloroglucin. Dilospan S. Spasfon-Lyoc



CAS Registry Number: 108-73-6

Related CAS Registry Numbers(s): 6099-90-7

Molecular Formula: C₆H₆O₃

Molecular Weight: 126.112

Accurate Mass: 126.031695

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Source: Isol. from *Eucalyptus kino* and *Acacia arabica*

Use/Importance: Spasmolytic agent, used as mixt. with trimethyl ether. Anal. reagent used for the detn. of aldehydes. Used in diazo-type-copying and textile-dyeing

Physical Description: Leaflets or plates + 2H₂O (H₂O)

Melting Point: Mp 117° (dihydrate). Mp 217-219° (anhyd.) (rapid heat). Mp 200-209° (slow heat)

Solubility: Mod. sol. H₂O; sol. EtOH, Et₂O, Py, Me₂CO

pKa Value: pK_{a1} 7.97; pK_{a2} 9.23 (20°)

Calculated Log P Data: Log P 0.14 (calc)

Other Data: Forms polymers with aldehydes and with diamines; no coml. importance

Hazard & Toxicity: Skin and eye irritant. LD₅₀ (rat, orl) 5200 mg/kg. Exp. reprod. effects

Fluka: 79330

>>Derivative: Tri-Ac

CAS Registry Number: 2999-40-8

Molecular Formula: C₁₂H₁₂O₆

Molecular Weight: 252.223

Accurate Mass: 252.06339

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Physical Description: Cryst.

Melting Point: Mp 104°

>>Derivative: Tribenzoyl

CAS Registry Number: 7510-54-5

Molecular Formula: C₂₇H₁₈O₆

Molecular Weight: 438.436

Accurate Mass: 438.11034

Percentage Composition: C 73.97%; H 4.14%; O 21.90%

Physical Description: Cryst.

Melting Point: Mp 185°

>>Derivative: Mono-Me ether

Synonym(s): 5-Methoxy-1,3-benzenediol, 9CI. 5-Methoxyresorcinol, 8CI. 3,5-Dihydroxyanisole. **Flamenol**, INN

CAS Registry Number: 2174-64-3

Molecular Formula: C₇H₈O₃

Molecular Weight: 140.138

Accurate Mass: 140.047345

Percentage Composition: C 60.00%; H 5.75%; O 34.25%

Use/Importance: Spasmolytic agent

Melting Point: Mp 78-81°

Boiling Point: Bp₁₆ 213°

Solubility: Sl. sol. H₂O, C₆H₆; sol. EtOH, Et₂O

Calculated Log P Data: Log P 0.96 (calc)

Aldrich: 23249-1

Fluka: 37478