



>>Entry Name: Phenylmethanetriol, 9Cl

Synonym(s): Orthobenzoic acid.  $\alpha$ -Trihydroxytoluene

CAS Registry Number: 498-68-0

PhC(OH)<sub>3</sub>

Molecular Formula: C<sub>7</sub>H<sub>8</sub>O<sub>3</sub>

Molecular Weight: 140.138

Accurate Mass: 140.047345

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

>>Derivative: Tri-Me ether

Synonym(s): Trimethoxymethylbenzene, 9Cl. Trimethyl orthobenzoate, 8Cl

CAS Registry Number: 707-07-3

Molecular Formula: C<sub>10</sub>H<sub>14</sub>O<sub>3</sub>

Molecular Weight: 182.219

Accurate Mass: 182.094295

Percentage Composition: C 65.92%; H 7.74%; O 26.34%

Physical Description: Liq.

Boiling Point: Bp 183-199°. Bp<sub>25</sub> 114-115°

Aldrich: 16453-4

>>Derivative: Tri-Et ether

Synonym(s): Triethoxymethylbenzene, 9Cl. Triethyl orthobenzoate, 8Cl

CAS Registry Number: 1663-61-2

Molecular Formula: C<sub>13</sub>H<sub>20</sub>O<sub>3</sub>

Molecular Weight: 224.299

Accurate Mass: 224.141245

Percentage Composition: C 69.61%; H 8.99%; O 21.40%

Physical Description: Liq.

Boiling Point: Bp 240°. Bp<sub>8</sub> 106-109°

Aldrich: 27085-7

Fluka: 75570

Sigma: T4899

>>Derivative: Tributyl ether

Synonym(s): Tributoxymethylbenzene, 9Cl. Tributyl orthobenzoate, 8Cl

CAS Registry Number: 49758-87-4

Molecular Formula: C<sub>19</sub>H<sub>32</sub>O<sub>3</sub>

Molecular Weight: 308.46

Accurate Mass: 308.235145

Percentage Composition: C 73.98%; H 10.46%; O 15.56%

Physical Description: Liq.

Boiling Point: Bp<sub>13</sub> 146-150°

#### References:

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Post, H.W., *Chemistry of Aliphatic Orthoesters*, Reinhold, New York, 1943, (*rev*)

McElvain, S.M. *et al.*, *J.A.C.S.*, 1950, **72**, 1661, (*synth*)

Schroll, G. *et al.*, *Ark. Kemi*, 1966, **26**, 279, (*ms*)

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