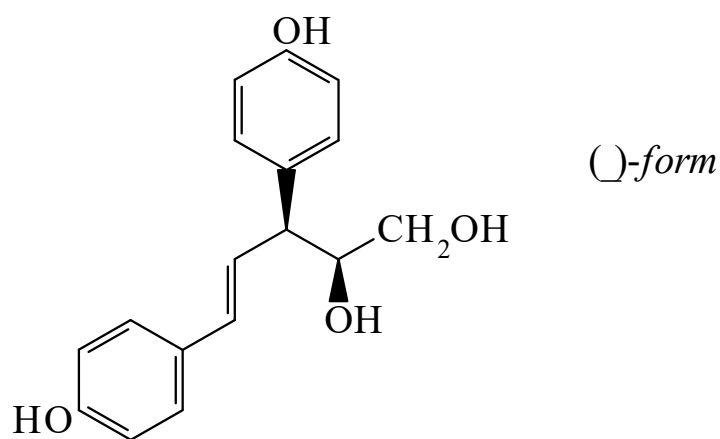




>>Entry Name: Agatharesinol

Synonym(s): 3,5-Bis(4-hydroxyphenyl)-4-pentene-1,2-diol, 9Cl



CAS Registry Number: 7288-11-1

Molecular Formula: C<sub>17</sub>H<sub>18</sub>O<sub>4</sub>

Molecular Weight: 286.327

Accurate Mass: 286.12051

Percentage Composition: C 71.31%; H 6.34%; O 22.35%

>>Variant: (-)-form

Molecular Formula: C<sub>17</sub>H<sub>18</sub>O<sub>4</sub>

Molecular Weight: 286.327

Accurate Mass: 286.12051

Percentage Composition: C 71.31%; H 6.34%; O 22.35%

Biological Source: Constit. of the heartwood of *Sequoia* spp., *Cryptomeria japonica*, *Agathis australis* and *Anthrotaxis selaginoides*

Physical Description: Cryst. (formerly descr. as a resin)

Melting Point: Mp 105-109°

Optical Rotation:  $[\alpha]_D^{25} -37.6$  (c, 1.7 in Me<sub>2</sub>CO)

>>Derivative: Tetra-Ac

CAS Registry Number: 7287-90-3

Molecular Formula: C<sub>25</sub>H<sub>26</sub>O<sub>8</sub>

Molecular Weight: 454.476

Percentage Composition: C 66.07%; H 5.77%; O 28.16%

Physical Description: Resin

Optical Rotation:  $[\alpha]_D -19$  (c, 1 in CHCl<sub>3</sub>)

>>Variant: (±)-form

Molecular Formula: C<sub>17</sub>H<sub>18</sub>O<sub>4</sub>

Molecular Weight: 286.327

Accurate Mass: 286.12051

Percentage Composition: C 71.31%; H 6.34%; O 22.35%

>>Derivative: 4',4''-Di-Me ether

CAS Registry Number: 61171-98-0

Molecular Formula: C<sub>19</sub>H<sub>22</sub>O<sub>4</sub>

Molecular Weight: 314.38

Percentage Composition: C 72.59%; H 7.05%; O 20.36%

Physical Description: Cryst. (CHCl<sub>3</sub> or MeOH)

Melting Point: Mp 124-126°

References:

- Enzell, C.R. *et al.*, *Acta Chem. Scand.*, 1965, **19**, 913, (*isol, struct*)  
Enzell, C.R. *et al.*, *Tet. Lett.*, 1966, 2395; 1967, 221; 793, (*struct, ms, abs config*)  
Daniels, P. *et al.*, *Chem. Comm.*, 1972, 246, (*isol*)  
Beraciertia, A.P. *et al.*, *J.C.S. Perkin I*, 1978, 1257, (*synth*)  
Muraoka, O. *et al.*, *J.C.S. Perkin I*, 1996, 405, (*synth*)  
Chen, X.H. *et al.*, *Z. Naturforsch., C*, 2001, **56**, 249-252, (*isol, pmr, cmr*)