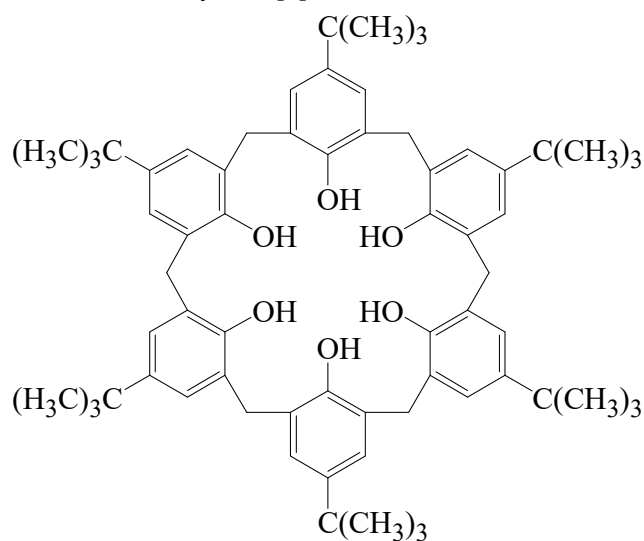




>>Entry Name: 5,11,17,23,29,35-Hexa-*tert*-butylcalix[6]arene-37,38,39,40,41,42-hexol

Synonym(s): 5,11,17,23,29,35-Hexakis(1,1-dimethylethyl)heptacyclo[31.3.1.1^{3,7}.1^{9,13}.1^{15,19}.1^{21,25}.1^{27,31}]dotetraconta-1(37),3,5,7(42),9,11,13(41),15,17,19(40),21,23,25(39),27,29,31(38),33,35-octadecaene-37,38,39,40,41,42-hexol, 9Cl. 4-*tert*-Butylcalix[6]arenehexol



CAS Registry Number: 78092-53-2

Related CAS Registry Numbers(s): 122742-65-8 136202-82-9 138709-55-4 140149-06-0 149472-72-0 149472-73-1 149472-74-2 149472-75-3 149472-76-4 149472-77-5 149772-36-1 151803-43-9 154388-72-4 154388-73-5

Molecular Formula: C₆₆H₈₄O₆

Molecular Weight: 973.386

Accurate Mass: 972.62679

Percentage Composition: C 81.44%; H 8.70%; O 9.86%

Use/Importance: Forms inclusion compds. with metal ions and small organic molecules. Intermed. to metal ion-selective complexing agent

Physical Description: Glistening cryst. (CHCl₃/MeOH)

Melting Point: Mp 380-381° (as CHCl₃/MeOH solvate)

pKa Value: pK_a 3.62 (25°, THF)

Other Data: Many mono-, di-, tri- and tetra-substituted ethers and acetates also known

Aldrich: 36369-3

>>Derivative: Hexa-Ac

CAS Registry Number: 78077-35-7

Molecular Formula: C₇₈H₉₆O₁₂

Molecular Weight: 1225.609

Accurate Mass: 1224.69018

Percentage Composition: C 76.44%; H 7.89%; O 15.67%

Physical Description: Cryst. (CHCl₃/MeOH)

Melting Point: Mp 360-362°

>>Derivative: Hexa-Me ether

CAS Registry Number: 98127-73-2

Molecular Formula: C₇₂H₉₆O₆

Molecular Weight: 1057.547

Accurate Mass: 1056.72069

Percentage Composition: C 81.77%; H 9.15%; O 9.08%

Physical Description: Cryst. + 1MeOH

Melting Point: Mp 210-213°. Mp 315-317° (dec.)

References:

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