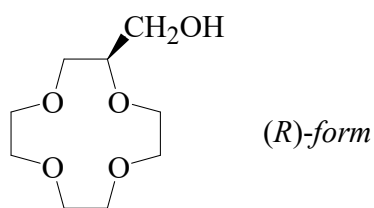




>>Entry Name: **2-(Hydroxymethyl)-12-crown-4**

Synonym(s): 1,4,7,10-Tetraoxacyclododecane-2-methanol, 9CI



CAS Registry Number: 75507-26-5

Molecular Formula: C₉H₁₈O₅

Molecular Weight: 206.238

Accurate Mass: 206.115425

Percentage Composition: C 52.41%; H 8.80%; O 38.79%

Use/Importance: Intermed. for the synth. of modified crown ethers

Aldrich: 38265-5

Fluka: 55629

>>Variant: (R)-form

CAS Registry Number: 122804-81-3

Molecular Formula: C₉H₁₈O₅

Molecular Weight: 206.238

Accurate Mass: 206.115425

Percentage Composition: C 52.41%; H 8.80%; O 38.79%

Boiling Point: Bp_{0.1} 115-117°

Optical Rotation: [α]_D -26.7 (neat)

>>Derivative: Ac

CAS Registry Number: 146609-61-2

Molecular Formula: C₁₁H₂₀O₆

Molecular Weight: 248.275

Accurate Mass: 248.12599

Percentage Composition: C 53.22%; H 8.12%; O 38.67%

Optical Rotation: [α]_D²¹ -6.7 (c, 1.28 in CHCl₃)

>>Variant: (S)-form

CAS Registry Number: 122770-12-1

Molecular Formula: C₉H₁₈O₅

Molecular Weight: 206.238

Accurate Mass: 206.115425

Percentage Composition: C 52.41%; H 8.80%; O 38.79%

Boiling Point: Bp_{0.1} 115-120°

Optical Rotation: [α]_D +31.9 (neat)

>>Derivative: Ac

CAS Registry Number: 146609-60-1

Molecular Formula: C₁₁H₂₀O₆

Molecular Weight: 248.275

Percentage Composition: C 53.22%; H 8.12%; O 38.67%

Optical Rotation: [α]_D²¹ +6.7 (c, 1.11 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 149561-75-1

Molecular Formula: C₉H₁₈O₅

Molecular Weight: 206.238

Accurate Mass: 206.115425

Percentage Composition: C 52.41%; H 8.80%; O 38.79%

Boiling Point: Bp_{0.04} 115°

Density: d 1.19

Refractive Index: n_D²⁰ 1.4806

References: