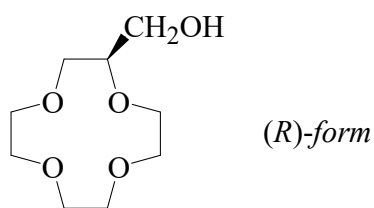




>>Entry Name: 2-(Hydroxymethyl)-12-crown-4

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



CAS Registry Number: 75507-26-5

Molecular Formula: $C_9H_{18}O_5$

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: $C_9H_{18}O_5$

Molecular Weight: 206.238

Accurate Mass: 206.115425

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

Boiling Point: $B_{p0.1}$ 115-117°

Optical Rotation: $[\alpha]_D -26.7$ (neat)

>>Derivative: Ac

CAS Registry Number: 146609-61-2

Molecular Formula: $C_{11}H_{20}O_6$

Molecular Weight: 248.275

Accurate Mass: 248.12599

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

Optical Rotation: $[\alpha]_D^{21} -6.7$ (c, 1.28 in $CHCl_3$)

>>Variant: (S)-form

CAS Registry Number: 122770-12-1

Molecular Formula: $C_9H_{18}O_5$

Molecular Weight: 206.238

Accurate Mass: 206.115425

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

Boiling Point: $B_{p0.1}$ 115-120°

Optical Rotation: $[\alpha]_D +31.9$ (neat)

>>Derivative: Ac

CAS Registry Number: 146609-60-1

Molecular Formula: $C_{11}H_{20}O_6$

Molecular Weight: 248.275

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

Optical Rotation: $[\alpha]_D^{21} +6.7$ (c, 1.11 in $CHCl_3$)

>>Variant: (±)-form

CAS Registry Number: 149561-75-1

Molecular Formula: $C_9H_{18}O_5$

Molecular Weight: 206.238

Accurate Mass: 206.115425

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

Boiling Point: $B_{p0.04}$ 115°

Density: d 1.19

Refractive Index: n_D^{20} 1.4806

References: