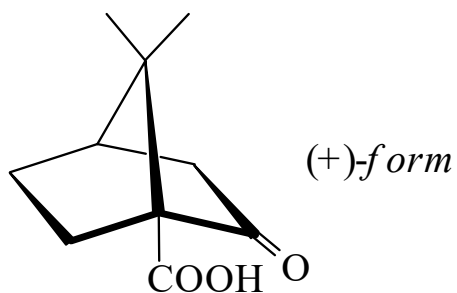




>>Entry Name: 7,7-Dimethyl-2-oxobicyclo[2.2.1]heptane-1-carboxylic acid

Synonym(s): Ketopinic acid



CAS Registry Number: 464-78-8

Extra CAS Registry Numbers(s): 6994-94-1

Molecular Formula: $C_{10}H_{14}O_3$

Molecular Weight: 182.219

Accurate Mass: 182.094295

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

Use/Importance: Useful resolving agent

Aldrich: 42096-4

Fluka: 60722

>>Variant: (+)-form

CAS Registry Number: 40724-67-2

Molecular Formula: $C_{10}H_{14}O_3$

Molecular Weight: 182.219

Accurate Mass: 182.094295

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

Physical Description: Cryst. (H_2O)

Melting Point: Mp 226-228°

Optical Rotation: $[\alpha]_D +25.8$ (c, 0.65 in MeOH)

>>Derivative: Amide

Synonym(s): Ketopinamide

CAS Registry Number: 136087-99-5

Molecular Formula: $C_{10}H_{15}NO_2$

Molecular Weight: 181.234

Accurate Mass: 181.110279

Percentage Composition: C 66.27%; H 8.34%; N 7.73%; O 17.66%

Physical Description: Spears (Et_2O /petrol)

Melting Point: Mp 192-195°

Optical Rotation: $[\alpha]_D +116.4$ (c, 0.75 in $CHCl_3$)

>>Variant: (–)-form

CAS Registry Number: 64234-14-6

Molecular Formula: $C_{10}H_{14}O_3$

Molecular Weight: 182.219

Accurate Mass: 182.094295

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

Physical Description: Cryst. (H_2O)

Melting Point: Mp 227-229°

Optical Rotation: $[\alpha]_D -28$ (c, 1.5 in MeOH)

>>Derivative: Chloride

Molecular Formula: $C_{10}H_{13}ClO_2$

Molecular Weight: 200.664

Accurate Mass: 200.060407

Percentage Composition: C 59.86%; H 6.53%; Cl 17.67%; O 15.95%

Use/Importance: Resolving agent

Melting Point: Mp 112°

Optical Rotation: $[\alpha]_D -41$ (c, 1.9 in $CHCl_3$)

References: