



>>Entry Name: 3,5,5-Trimethylhexanoic acid, 9Cl

Synonym(s): Isononanoic acid‡

CAS Registry Number: 3302-10-1

$(\text{H}_3\text{C})_3\text{CCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_9\text{H}_{18}\text{O}_2$

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Rare Chemicals Library: S41500-6

>>Variant: (±)-form

Molecular Formula: $\text{C}_9\text{H}_{18}\text{O}_2$

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Physical Description: Liq.

Boiling Point: Bp_{10} 121°. Bp_4 85°

Refractive Index: n_D^{25} 1.4268

>>Derivative: Et ester

CAS Registry Number: 67707-75-9

Molecular Formula: $\text{C}_{11}\text{H}_{22}\text{O}_2$

Molecular Weight: 186.294

Accurate Mass: 186.16198

Percentage Composition: C 70.92%; H 11.90%; O 17.18%

Physical Description: Liq.

Boiling Point: Bp_{35} 103°

Refractive Index: n_D^{20} 1.4177

>>Derivative: Chloride

CAS Registry Number: 36727-29-4

Molecular Formula: $\text{C}_9\text{H}_{17}\text{ClO}$

Molecular Weight: 176.685

Accurate Mass: 176.096792

Percentage Composition: C 61.18%; H 9.70%; Cl 20.07%; O 9.06%

Physical Description: Liq.

Boiling Point: Bp 188-190°

Density: d 0.93

Refractive Index: n_D^{20} 1.4360

Aldrich: 42295-9

>>Derivative: Amide

CAS Registry Number: 90726-43-5

Molecular Formula: $\text{C}_9\text{H}_{19}\text{NO}$

Molecular Weight: 157.255

Accurate Mass: 157.146664

Percentage Composition: C 68.74%; H 12.18%; N 8.91%; O 10.17%

Physical Description: Cryst.

Melting Point: Mp 96°

>>Derivative: Nitrile

CAS Registry Number: 3378-75-4

Molecular Formula: $\text{C}_9\text{H}_{17}\text{N}$

Molecular Weight: 139.24

Accurate Mass: 139.136099

Percentage Composition: C 77.64%; H 12.31%; N 10.06%

Physical Description: Liq.

Boiling Point: Bp 194-195°. Bp_{10} 110°

Refractive Index: n_D^{25} 1.4225