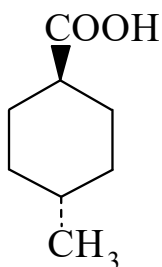




>>Entry Name: 4-Methylcyclohexanecarboxylic acid



(1*RS*,4*RS*)-form

CAS Registry Number: 4331-54-8

Molecular Formula: C₈H₁₄O₂

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Aldrich: 33062-0

>>Variant: (1*RS*,4*RS*)-form

Synonym(s): *trans*-form

CAS Registry Number: 13064-83-0

Molecular Formula: C₈H₁₄O₂

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Physical Description: Cryst. (formic acid)

Melting Point: Mp 110.5-111.5°

pKa Value: p*K*_a 4.89 (25°)

>>Derivative: Me ester

CAS Registry Number: 29886-34-8

Molecular Formula: C₉H₁₆O₂

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Boiling Point: Bp 192-194°. Bp₁₃ 74-75°

>>Derivative: 4-Bromophenacyl ester

Melting Point: Mp 136-136.5°

>>Derivative: Amide

CAS Registry Number: 60940-94-5

Molecular Formula: C₈H₁₅NO

Molecular Weight: 141.213

Accurate Mass: 141.115364

Percentage Composition: C 68.04%; H 10.71%; N 9.92%; O 11.33%

Physical Description: Plates (H₂O)

Melting Point: Mp 226°

>>Derivative: Nitrile

Synonym(s): 1-Cyano-4-methylcyclohexane

CAS Registry Number: 40636-31-5

Molecular Formula: C₈H₁₃N

Molecular Weight: 123.197

Accurate Mass: 123.104799

Percentage Composition: C 78.00%; H 10.64%; N 11.37%

Boiling Point: Bp₁₈ 85-87°

>>Variant: (1*RS*,4*SR*)-form

Synonym(s): *cis*-form