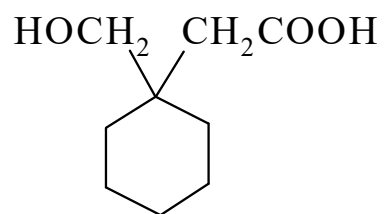




>>Entry Name: 1-(Hydroxymethyl)cyclohexaneacetic acid, 9CI

Synonym(s): 3,3-Pentamethylene-4-hydroxybutyric acid. Hexacyclonic acid



CAS Registry Number: 7491-42-1

Molecular Formula: C₉H₁₆O₃

Molecular Weight: 172.224

Accurate Mass: 172.109945

Percentage Composition: C 62.77%; H 9.36%; O 27.87%

Use/Importance: Central stimulant

Calculated Log P Data: Log P 0.95 (calc)

>>Derivative: Na salt

Synonym(s): Hexacyclonate sodium, INN. Gevilon‡. Neuryl. Repriscal. W 1597

CAS Registry Number: 7009-49-6

Physical Description: Plates (butanol/C₆H₆)

Melting Point: Mp 106-108° (monohydrate)

Hazard & Toxicity: LD₅₀ (rat, orl) 20 mg/kg

References:

U.S. Pat., 1960, *Warner-Lambert*, 3 007 940; *CA*, **56**, 8591g, (*synth, pharmacol*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., *Van Nostrand Reinhold*, 1992, SHL500