



>>Entry Name: 2,4-Cyclopentadien-1-ylsodium, 9CI

Synonym(s): Sodium cyclopentadienide



CAS Registry Number: 4984-82-1

Molecular Formula: C₅H₅Na

Molecular Weight: 88.084

Accurate Mass: 88.028892

Percentage Composition: C 68.18%; H 5.72%; Na 26.10%

General Statement: Multidecker struct. in the solid state with each metal atom linearly coord. by two η^5 -bonded Cp rings

Source/Synthesis: Synth. from CpH and Na or NaH

Use/Importance: Reagent for synth. of cyclopentadienyl compds. Adds to pyrylium salts. Substitutes esters, carbonates; substitutes allyl acetates in the presence of Pd(dppe)₂

Physical Description: Colourless cryst.

Solubility: Sol. ethers

Other Data: Forms complexes with ethers, amines. Dec. >300°

Hazard & Toxicity: Pyrophoric in air

Aldrich: 30402-6

Fluka: 29675

>>Derivative: TMED complex

CAS Registry Number: 59828-67-0

Molecular Formula: C₁₁H₂₁N₂Na

Molecular Weight: 204.29

Percentage Composition: C 64.67%; H 10.36%; N 13.71%; Na 11.25%

Physical Description: Plates (C₆H₆)

Melting Point: Mp 135-138°

Solubility: Sol. THF; spar. sol. C₆H₆, toluene

>>Derivative: DME complex

CAS Registry Number: 62228-16-4

Molecular Formula: C₉H₁₅NaO₂

Molecular Weight: 178.206

Percentage Composition: C 60.66%; H 8.48%; Na 12.90%; O 17.96%

Source/Synthesis: Synth. from CpH and Na in DME

Physical Description: White powder

Solubility: Sol. THF; insol. toluene

Other Data: Less air-sensitive and more easily handled than uncomplexed CpNa

References:

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