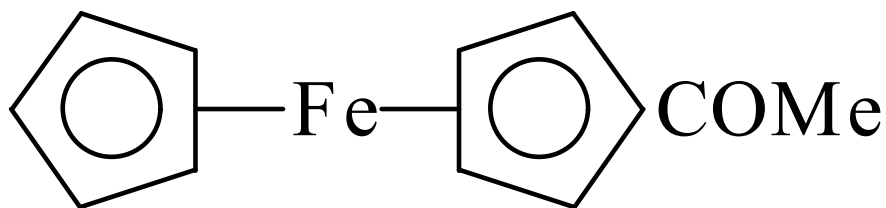




>>Entry Name: Acetylferrocene, 9CI

Synonym(s): Ferrocenyl methyl ketone



CAS Registry Number: 1271-55-2

Related CAS Registry Numbers(s): 12193-78-1

Molecular Formula: $C_{12}H_{12}FeO$

Molecular Weight: 228.073

Accurate Mass: 228.023754

Percentage Composition: C 63.20%; H 5.30%; Fe 24.49%; O 7.02%

Source/Synthesis: Synth. from ferrocene and acetic anhydride with various catalysts

Use/Importance: Curing agent in resin production; reduces flammability and suppresses smoke production in pvc

Physical Description: Orange cryst. (heptane)

Melting Point: Mp 85-86°

pKa Value: $pK_{a1} -2.8$ (H_2SO_4 aq.)

NMR Spectra: Pmr 2.28 (CH_3) ppm

Other Data: Exhibits phase transitions at 80° and 3°

Hazard & Toxicity: LD₅₀ (oral, female rats) <5 mg/kg, (oral, male rats) <50 mg/kg, (oral, monkeys) <100 mg/kg

Aldrich: 10686-0

Fluka: 1130

Sigma: A1011

>>Derivative: (E)-Oxime

CAS Registry Number: 32662-56-9

Molecular Formula: $C_{12}H_{13}FeNO$

Molecular Weight: 243.088

Accurate Mass: 243.034653

Percentage Composition: C 59.29%; H 5.39%; Fe 22.97%; N 5.76%; O 6.58%

Physical Description: Orange-yellow flakes (hexane)

Melting Point: Mp 174-175°

>>Derivative: (Z)-Oxime

CAS Registry Number: 32662-57-0

Physical Description: Orange-yellow flakes (hexane)

Melting Point: Mp 144-145°