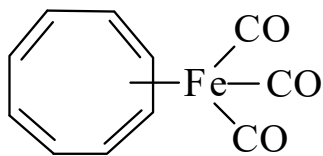




>>Entry Name: Tricarbonyl[(1,2,3,4- η)-1,3,5,7-cyclooctatetraene]iron, 9CI

Synonym(s): (η^4 -Cyclooctatetraene)tricarbonyliron



CAS Registry Number: 12093-05-9

Molecular Formula: $C_{11}H_8FeO_3$

Molecular Weight: 244.029

Accurate Mass: 243.982284

Percentage Composition: C 54.14%; H 3.30%; Fe 22.89%; O 19.67%

Source/Synthesis: Synth. from cot + $Fe(CO)_5$ or $Fe_3(CO)_{12}$

Physical Description: Deep-red needles (EtOH)

Melting Point: Mp 92-93.5°

Boiling Point: Subl._{0.1} 50°

Other Data: Ir ν_{CO} 2046, 2024, 1984, 1961, 1945 cm^{-1} (KBr)

Aldrich: 27591-3

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **3**, 777B, (*nmr*)

Manuel, T.A. *et al.*, *J.A.C.S.*, 1960, **82**, 366, (*synth*)

Dickens, B. *et al.*, *J.A.C.S.*, 1961, **83**, 4862, (*cryst struct*)

Fritz, H.P. *et al.*, *Chem. Ber.*, 1962, **95**, 158, (*ir, uv*)

Davison, A. *et al.*, *J.C.S.*, 1962, 4821, (*synth*)

Organomet. Synth., 1965, **1**, 126, (*synth*)

Inorg. Synth., 1966, **8**, 184, (*synth*)

King, R.B., *Appl. Spectrosc.*, 1969, **23**, 536; *CA*, **71**, 117665, (*ms*)

Cotton, F.A. *et al.*, *J.A.C.S.*, 1976, **98**, 1413, (*cmr*)

Behrens, H. *et al.*, *J. Organomet. Chem.*, 1980, **192**, 389, (*pmr*)