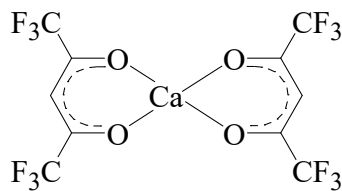




>>Entry Name: Bis(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-*O,O'*)calcium(II)

Synonym(s): Bis(hexafluoroacetylacetonato)calcium. Calcium hexafluoroacetylacetonate. Ca(hfac)₂



CAS Registry Number: 121012-90-6

Molecular Formula: C₁₀H₂CaF₁₂O₄

Molecular Weight: 454.182

Accurate Mass: 453.938737

Percentage Composition: C 26.45%; H 0.44%; Ca 8.82%; F 50.20%; O 14.09%

General Statement: Anhyd. compd. is probably oligomeric

Source/Synthesis: Synth. from Ca + CF₃COCH₂COCF₃

Use/Importance: Used in the deposition of CaF₂ by low-pressure MOCVD

Physical Description: Sl. yellow powder

Melting Point: Mp 170-230°

Boiling Point: Bp_{0.07} 180°

Other: Gelest AKC163

>>Derivative: Dihydrate

CAS Registry Number: 141572-90-9

Extra CAS Registry Numbers(s): 141624-18-2

Molecular Formula: C₁₀H₆CaF₁₂O₆

Molecular Weight: 490.213

Accurate Mass: 489.959867

Percentage Composition: C 24.50%; H 1.23%; Ca 8.18%; F 46.51%; O 19.58%

Physical Description: Cryst. (Et₂O/petrol)

Other Data: Dimeric

>>Derivative: Tetraglyme complex (2:1)

CAS Registry Number: 140656-02-6

Extra CAS Registry Numbers(s): 144472-51-5 153111-39-8

Molecular Formula: C₃₀H₂₆Ca₂F₂₄O₁₃

Molecular Weight: 1130.645

Accurate Mass: 1130.024199

Percentage Composition: C 31.87%; H 2.32%; Ca 7.09%; F 40.33%; O 18.40%

Use/Importance: Precursor in MOCVD

Physical Description: Air-stable cryst.

Melting Point: Mp 94-95°

References:

Purdy, A.P. *et al.*, *Inorg. Chem.*, 1989, **28**, 2799-2803, (*synth, ir, pmr, F-19 nmr, ms*)

Bradley, D.C. *et al.*, *Chem. Comm.*, 1992, 575-576, (*dihydrate, cryst struct*)

Drake, S.R. *et al.*, *Inorg. Chem.*, 1993, **32**, 3227-3335, (*tetraglyme complex, synth, ir, pmr, cmr, ms, cryst struct*)

Inorg. Synth., 1997, **31**, 1-7, (*synth, pmr*)