



>>Entry Name: **Tris(2,2,6,6-tetramethyl-3,5-heptanedionato-*O,O'*)gadolinium(III)**

Synonym(s): Tris(dipivaloylmethanido)gadolinium. Resolve-Al Gd. Gd(thd)₃

CAS Registry Number: 14768-15-1

As Tris(2,2,6,6-tetramethyl-3,5-heptanedionato-*O,O'*)chromium(III), [HXL76-F](#) with
M = Gd

Molecular Formula: C₃₃H₅₇GdO₆

Molecular Weight: 707.06

Accurate Mass: 707.339614

Percentage Composition: C 56.06%; H 8.13%; Gd 22.24%; O 13.58%

Use/Importance: Commercially available. Nmr shift reagent. Used as a spin label in ¹⁵N nmr

Aldrich: 23729-9

Sigma: T3017

Other: Gelest AKG306

>>Derivative: Hydrate

Molecular Formula: C₃₃H₅₉GdO₇

Molecular Weight: 725.075

Accurate Mass: 725.350179

Percentage Composition: C 54.67%; H 8.20%; Gd 21.69%; O 15.45%

Source/Synthesis: Obt. from GdCl₃, tmhdH (tmhd = 2,2,6,6-tetramethyl-3,5-heptanedionato) and NaOH in MeOH

Physical Description: Off-white solid

Solubility: Sol. MeOH

>>Derivative: Dimer

Molecular Formula: C₆₆H₁₁₄Gd₂O₁₂

Molecular Weight: 1414.119

Accurate Mass: 1414.679228

Percentage Composition: C 56.06%; H 8.13%; Gd 22.24%; O 13.58%

Source/Synthesis: Obt. on cryst. of hydrate from hexane

Physical Description: Hygroscopic white needles

Melting Point: Mp 171-172°. Mp 182-184°

Boiling Point: Subl. 110-148° (0.00005 mm)

Solubility: Sol. C₆H₆, CHCl₃, MeOH, EtOH, CCl₄, EtOAc, hexane

Other Data: Paramagnetic, $\mu_{\text{eff}} = 7.6, 7.8\mu_{\text{B}}$. Dimer has Gd bound to two terminal tmhd and one bridging tmhd; 7-coord. Gd in distorted monocapped trigonal prismatic arrangement

>>Derivative: Py complex

Synonym(s): (Pyridine)tris(2,2,6,6-tetramethyl-3,5-heptanedionato-*O,O'*)gadolinium(III)

CAS Registry Number: 33134-16-6

Molecular Formula: C₃₈H₆₂GdNO₆

Molecular Weight: 786.161

Accurate Mass: 786.381813

Percentage Composition: C 58.06%; H 7.95%; Gd 20.00%; N 1.78%; O 12.21%

Physical Description: White cryst.

Melting Point: Mp 134-135°

Solubility: Sol. Py, C₆H₆

Other Data: Paramagnetic, $\mu_{\text{eff}} = 7.8\mu_{\text{B}}$

>>Derivative: Bipy complex

Synonym(s): (2,2'-Bipyridine-*N,N'*)tris(2,2,6,6-tetramethyl-3,5-heptanedionato-*O,O'*)gadolinium(III)

CAS Registry Number: 33134-17-7

Molecular Formula: C₄₃H₆₅GdN₂O₆

Molecular Weight: 863.246

Accurate Mass: 863.408362

Percentage Composition: C 59.83%; H 7.59%; Gd 18.22%; N 3.25%; O 11.12%

Physical Description: White cryst.

Melting Point: Mp 192-193°

Solubility: Sol. Py, hexane

Other Data: Paramagnetic, $\mu_{\text{eff}} = 7.9\mu_{\text{B}}$