



>>Entry Name: 4,4,4-Trifluoro-1-(2-thienyl)-1,3-butanedione

Synonym(s): Thenoyltrifluoroacetone. HTTA



CAS Registry Number: 326-91-0

Molecular Formula: C₈H₅F₃O₂S

Molecular Weight: 222.187

Accurate Mass: 221.996234

Percentage Composition: C 43.25%; H 2.27%; F 25.65%; O 14.40%; S 14.43%

Use/Importance: Forms chelate complexes with lanthanide and actinide elements, which are useful in their isolation, separation and estimation. Used as 0.15M C₆H₆ soln. or 0.5M soln. in xylene for extraction separation of Cr(III), Fe(III), Mn, Sc, Zn, Ca, Pu(VI), Tl(III), Ti, V, Zr; photometric detn. of Ce(IV) ($\lambda_{\max}$ 450 nm, ϵ 2500), Co, Ga, In, Pd; extraction-photometric detn. of Fe(II), Ir, Pu(VI)

Physical Description: Cryst.

Melting Point: Mp 42.5-43.2°

Boiling Point: Bp₈ 96-98°

pKa Value: pK_{a1} 6.53 (25°, μ = 1.0)

Aldrich: T2700-6

Fluka: 88300

Rare Chemicals Library: S26445-8

Sigma: T9888

>>Derivative: Oxime

Molecular Formula: C₈H₆F₃NO₂S

Molecular Weight: 237.202

Accurate Mass: 237.007133

Percentage Composition: C 40.51%; H 2.55%; F 24.03%; N 5.90%; O 13.49%; S 13.52%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 134°

Other Data: Not known whether 1 or 3 oxime

>>Derivative: Cu complex

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 242-243°

References:

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Nash, K.L. *et al.*, *CA*, 1976, **85**, 52441u, (*detn, Zn*)
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