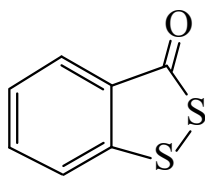




>>Entry Name: **3*H*-1,2-Benzodithiol-3-one**, 9Cl

Synonym(s): Dithiobenzoyl. Benzo[*c*]dithiol-3-one. 1,2-Benzodisulfol-3-one



CAS Registry Number: 1677-27-6

Molecular Formula: C₇H₄OS₂

Molecular Weight: 168.24

Accurate Mass: 167.970355

Percentage Composition: C 49.97%; H 2.40%; O 9.51%; S 38.12%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 78-80°

Aldrich: 37546-2

Fluka: 12343

>>Derivative: *S*¹-Oxide

CAS Registry Number: 127183-89-5

Molecular Formula: C₇H₄O₂S₂

Molecular Weight: 184.239

Accurate Mass: 183.96527

Percentage Composition: C 45.63%; H 2.19%; O 17.37%; S 34.81%

Physical Description: Cryst. (CH₂Cl₂/hexane)

Melting Point: Mp 103.5-104°

>>Derivative: *S*¹,*S*¹-Dioxide

Synonym(s): 3*H*-1,2-Benzodithiole-3-one 1,1-dioxide. Beaucage reagent

CAS Registry Number: 66304-01-6

Molecular Formula: C₇H₄O₃S₂

Molecular Weight: 200.239

Accurate Mass: 199.960185

Percentage Composition: C 41.99%; H 2.01%; O 23.97%; S 32.03%

Use/Importance: Sulfurizing reagent in oligodeoxyribonucleoside phosphorothioate synth.

Physical Description: Cryst. (CH₂Cl₂/hexane)

Melting Point: Mp 102.5-103° (98-99°)

Aldrich: 37547-0

Sigma: B8171

Other: Davos chemical corp.

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1305C, (*nmr*)

Smiles, S. *et al.*, *J.C.S.*, 1922, 86, (*synth*)

Raoul, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1959, 1670, (*synth*)

Boberg, F. *et al.*, *Annalen*, 1967, **708**, 148, (*ir, synth*)

Hortmann, A.G. *et al.*, *J.O.C.*, 1978, **43**, 3374, (*synth*)

Iyer, R.P. *et al.*, *J.O.C.*, 1990, **55**, 4693, (*oxides*)

Regan, J.B. *et al.*, *Org. Prep. Proced. Int.*, 1992, **24**, 488, (***synth***, *dioxide*)

Marchan, V. *et al.*, *Synthesis*, 1999, 43-45, (*synth, oxides, cmr, ms*)