



Molecular Weight: 128.154
Accurate Mass: 128.004433
Percentage Composition: C 37.49%; H 3.15%; N 21.86%; O 12.48%; S 25.02%
Other Data: Minor tautomer

>>**Derivative:** Me thioether

Synonym(s): 2-(Methylthio)-4(1*H*)-pyrimidinone

CAS Registry Number: 5751-20-2

Molecular Formula: C₅H₆N₂OS

Molecular Weight: 142.181

Accurate Mass: 142.020083

Percentage Composition: C 42.24%; H 4.25%; N 19.70%; O 11.25%; S 22.55%

Physical Description: Cryst.

Melting Point: Mp 199-201°

Rare Chemicals Library: S44004-3

>>**Derivative:** Et thioether

Synonym(s): 2-(Ethylthio)-4(1*H*)-pyrimidinone

CAS Registry Number: 6965-19-1

Molecular Formula: C₆H₈N₂OS

Molecular Weight: 156.208

Accurate Mass: 156.035733

Percentage Composition: C 46.13%; H 5.16%; N 17.93%; O 10.24%; S 20.53%

Physical Description: Cryst.

Melting Point: Mp 151-152°

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 820C, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 378A, (*nmr*)
Warrener, R.N. *et al.*, *Chem. Ind. (London)*, 1964, 1989, (*deriv*)
Croitoru, V. *et al.*, *CA*, 1968, **68**, 9076r, (*detn, Pd*)
IARC Monog., 1974, **7**, 85; *Suppl.* 7, 72, (*rev, tox*)
Yoshimura, M. *et al.*, *Yakugaku Zasshi*, 1976, **96**, 1094, (*synth*)
Maruizumi, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1978, **51**, 978, (*nmr*)
Still, I.W.J. *et al.*, *Can. J. Chem.*, 1978, **56**, 725, (*cmr*)
Hirota, K. *et al.*, *J.O.C.*, 1978, **43**, 1193, (*synth*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., *Pharmaceutical Press*, 1982, 840
Katritzky, A.R. *et al.*, *J.C.S. Perkin 2*, 1989, 1499; 1507; 1990, 871, (*pe, tautom, bibl*)
Spychala, J. *et al.*, *Synth. Commun.*, 1997, **27**, 1943-1949, (*S-Me*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., *Van Nostrand Reinhold*, 1992, TFR250