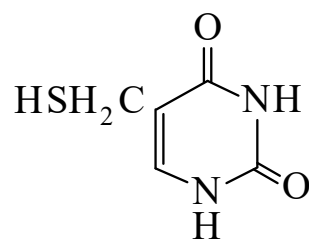




>>Entry Name: 5-(Mercaptomethyl)-2,4(1*H*,3*H*)-pyrimidinedione, 9Cl

Synonym(s): 5-Mercaptomethyluracil, 8Cl



CAS Registry Number: 4874-36-6

Molecular Formula: C₅H₆N₂O₂S

Molecular Weight: 158.181

Accurate Mass: 158.014998

Percentage Composition: C 37.97%; H 3.82%; N 17.71%; O 20.23%; S 20.27%

Use/Importance: Possesses tumour-inhibitory props.

Physical Description: Needles (MeOH)

Melting Point: Mp 272-274°

Calculated Log P Data: Log P -0.84 (uncertain value) (calc)

Other Data: Dec. at 315°

>>Derivative: S-Me

CAS Registry Number: 4874-40-2

Molecular Formula: C₆H₈N₂O₂S

Molecular Weight: 172.207

Accurate Mass: 172.030648

Percentage Composition: C 41.85%; H 4.68%; N 16.27%; O 18.58%; S 18.62%

Physical Description: Needles or prisms (MeOH)

Melting Point: Mp 258-260°

>>Derivative: S-Et

CAS Registry Number: 4874-41-3

Molecular Formula: C₇H₁₀N₂O₂S

Molecular Weight: 186.234

Accurate Mass: 186.046298

Percentage Composition: C 45.15%; H 5.41%; N 15.04%; O 17.18%; S 17.22%

Physical Description: Needles (MeOH)

Melting Point: Mp 244-246°

References:

Giner-Sorolla, A. *et al.*, *J. Med. Chem.*, 1966, **9**, 97, (*synth*)

Gupta, V.S. *et al.*, *J. Med. Chem.*, 1975, **18**, 973