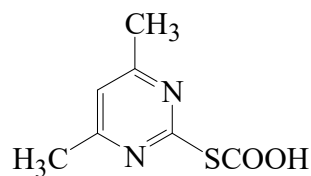




>>Entry Name: **S-(4,6-Dimethyl-2-pyrimidinyl)carbonothioic acid**, 9Cl



Molecular Formula: C₇H₈N₂O₂S

Molecular Weight: 184.218

Accurate Mass: 184.030648

Percentage Composition: C 45.64%; H 4.38%; N 15.21%; O 17.37%; S 17.41%

>>Derivative: *tert*-Butyl ester

Synonym(s): *O*-(1,1-Dimethylethyl) *S*-(4,6-dimethyl-2-pyrimidinyl)carbonothioate, 9Cl. *tert*-Butyl 4,6-dimethylpyrimidinyl-2-thiol carbonate. BOC S Reagent

CAS Registry Number: 41840-28-2

Molecular Formula: C₁₁H₁₆N₂O₂S

Molecular Weight: 240.326

Accurate Mass: 240.093248

Percentage Composition: C 54.98%; H 6.71%; N 11.66%; O 13.31%; S 13.34%

Use/Importance: Reagent for prep. of *tert*-BOC amino acids for peptide synth.

Physical Description: Cryst. (heptane)

Melting Point: Mp 50-51°

>>Derivative: 4-Methoxybenzyl ester

CAS Registry Number: 41840-29-3

Molecular Formula: C₁₅H₁₆N₂O₃S

Molecular Weight: 304.369

Accurate Mass: 304.088163

Percentage Composition: C 59.19%; H 5.30%; N 9.20%; O 15.77%; S 10.54%

Use/Importance: Reagent for prep. of 4-methoxybenzyloxycarbonyl (PM2) amino acids for peptide synthesis

Physical Description: Pale yellow cryst. (Et₂O/petrol)

Melting Point: Mp 58-60°

References:

Nagasawa, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 1269-1272, (*synth, use*)