

Synthesis of 7,8-dicyanopyrimido[2,1-*b*][1,3]benzothiazoles

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*Ethyl 7,8-dicyano-2-methyl-4-(4-methylphenyl)-4H-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxylate 4b.* Yield 72%, mp 236–238 °C (decomp.). IR (ν/cm^{-1}): 2232 (C≡N), 1685 (C=O), 1588 (C=C), 1586 (Ar), 1242 (C-O-C). MS, m/z (%): 414 [M^+] (21), 385 [M^+ - Et] (25), 341 [M^+ - COOEt] (100), 323 (62), 295 (30), 249 (28), 225 (42), 184 (27), 157 (12), 128 (18), 115 (45), 91 (24), 89 (15), 65 (38). ^1H NMR, δ : 1.21 (t, 3H, CH₃, J 7.3 Hz), 2.20 (s, 3H, 4'-CH₃), 2.33 (s, 3H, 2-CH₃), 4.06 (q, 2H, -CH₂-, J 7.3 Hz), 6.52 (s, 1H, 4-H), 7.12 (d, 2H, 3'-H, 5'-H, J 8.1 Hz), 7.39 (d, 2H, 2'-H, 6'-H, J 8.1 Hz), 8.26 (s, 1H, 9-H), 8.45 (s, 1H, 6-H). Found (%): C 66.58; H 4.16; N 13.43. Calc. for C₂₃H₁₈N₄O₂S (%): C 66.65; H 4.38; N 13.52.

*Ethyl 7,8-dicyano-4-(4-methoxyphenyl)-2-methyl-4H-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxylate 4c.* Yield 72%, mp 222–223 °C (decomp.). IR (ν/cm^{-1}): 2236 (C≡N), 1678 (C=O), 1606 (C=C), 1242 (C-O-C). MS, m/z (%): 430 [M^+] (20), 401 (18), 385 (5), 357 [M^+ - COOEt] (100), 323 (36), 295 (22), 249 (23), 225 (44), 184 (28), 157 (11), 115 (12), 77 (6). ^1H NMR, δ : 1.21 (t, 3H, CH₃, J 7.2 Hz), 2.33 (s, 3H, CH₃), 3.68 (s, 3H, OCH₃), 4.07 (d.q, 2H, -CH₂-, J 7.2 Hz), 6.52 (s, 1H, 4-H), 6.87 (d, 2H, 3'-H, 5'-H, J 8.8 Hz), 7.44 (d, 2H, 2'-H, 6'-H, J 8.8 Hz), 8.30 (s, 1H, 9-H), 8.46 (s, 1H, 6-H). Found (%): C 64.03; H 4.06; N 12.97. Calc. for C₂₃H₁₈N₄O₃S (%): C 64.17; H 4.21; N 13.01.

*Ethyl 7,8-dicyano-4-(4-methoxyphenyl)-2-phenyl-4H-pyrimido[2,1-*b*][1,3]benzothiazole-3-carboxylate 4e.* Yield 68%, mp 227–229 °C (decomp.). IR (ν/cm^{-1}): 2236 (C≡N), 1666 (C=O), 1609 (C=C), 1593 (Ar); 1241 (C-O-C). MS, m/z (%): 492 [M^+] (14), 463 [M^+ - Et] (6), 419 [M^+ - COOEt] (100), 385 (8), 300 (26), 287 (13), 92 (13), 77 (47). ^1H NMR, δ : 0.84 (t, 3H, CH₃, J 7.1 Hz), 3.71 (s, 3H, OMe), 3.82 (d.q, 2H, -CH₂-, J 7.1 Hz), 6.67 (s, 1H, 4-H), 6.93 (d, 2H, 3''-H, 5''-H, J 8.6 Hz), 7.39 (m, 5H, Ph), 7.54 (d, 2H, 2''-H, 6''-H, J 8.6 Hz), 8.35 (s, 1H, 6-H), 8.48 (s, 1H, 9-H). Found (%): C, 68.10; H, 3.96; N, 13.31. Calc. for C₂₈H₂₀N₄O₃S (%): C 68.28; H 4.09; N 11.37.