

Elimination of a Thiomethyl Substituent from an Anionic 5-Methylenebarbituric Acid Derivative by Oxidation and Substitution

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Z. Naturforsch. **2009**, *64b*, 307–312; received November 23, 2008

Dedicated to Professor Helmut Quast on the occasion of his 75th birthday

Triethylammonium 5-[(1,3-dimethyl-2,4,6-trioxo-tetrahydropyrimidin-5(6*H*)-ylidene)-(methylthio)methyl]-1,3-dimethyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-olate (**5**), obtained from 5-[bis(methylthio)methylene]-1,3-dimethyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione (**2**) and 1,3-dimethylbarbituric acid in the presence of triethylamine, is protonated by methanesulfonic acid to give 5,5'-(methylthiomethanediylidene)bis(1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione) (**6**) in good yield. Compound **6** is oxidized in two steps by *m*-chloroperbenzoic acid to give 5,5'-(methylsulfinylmethanediylidene)bis(1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione) (**7**) and 5-[(1,3-dimethyl-2,4,6-trioxo-tetrahydropyrimidin-5(6*H*)-ylidene)(methylsulfinyl)methyl]-5-hydroxy-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (**8**), respectively. Excess pyridine eliminates methanesulfonic acid from **8** to give the zwitterionic 5-[(1,3-dimethyl-2,4,6-trioxo-tetrahydropyrimidin-5(6*H*)-ylidene(pyridinium-1-yl)methyl]-1,3-dimethyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-olate (**9**). The crystal structures of compounds **6**, **8**, and **9** are reported.

Key words: Heterocycles, Barbituric Acid, Sulfur, Olefin, Crystal Structure