Derivate der 1,3-Dimethyl-5-methylene-barbitursäure

Derivatives of 1,3-Dimethyl-5-methylenebarbituric Acid

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1,3-Dimethylbarbituric acid (1, R = Me) reacts with aqueous formaldehyde in the presence of pyridine to give 1,3-dimethyl-2,4,6-trioxo-5-pyridinomethyl-1,3-perhydrodiazin-5-ylpyridinium ylide (6) in good yield. From 6 and 2,3-dihydro-1,3-diisopropyl-4,5-dimethylimidazol-2-ylidene (7), the zwitterionic imidazolium derivative 1,3-dimethyl-2,4,6-trioxo-5-(1,3-diisopropyl-4,5-dimethylimidazolomethyl)-1,3-perhydrodiazin-5-yl-imidazolium ylide (8) is obtained. Similarly, the phosphonium compound 1,3-dimethyl-2,4,6-trioxo-5-triphenylphosphoniomethyl-1,3-perhydrodiazin-5-yl-phosphonium ylide (9) is obtained from 6 and PPh₃. The crystal structures of 8 and 9 are reported.

Key words: Zwitterionic Compounds, Heterocycles, Imidazoles, Barbituric Acid, Crystal Structure