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Structure and intramolecular lability of N-(thio)phosphoryl(thio)amides: XIV. Electronic structure and spatial arrangement of N-[diisopropoxy(thio) phosphoryl](thio)benzamides

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Abstract

Semiempirical quantum-chemical calculations of the spatial arrangement and electronic structure of the tautomeric forms of N-[diisopropoxy(thio)phosphoryl] (thio)benzamides were carried out by the PM3 method. The most energetically favorable forms were revealed, and the reasons for their stabilization were discussed. © Pleiades Publishing, Inc. 2006.

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