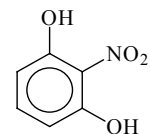


714  
ED $C_6H_5NO_4$ **1,3-Dihydroxy-2-nitrobenzene**  
2-Nitroresorcinol  
2-Nitro-1,3-benzenediol

The barrier height to the internal rotation of the nitro group was determined to be 34(2) kJ mol<sup>-1</sup> by the application of a dynamic model to the previous ED data using the Monte Carlo optimization method. The higher barrier than in nitrobenzene is a consequence of intramolecular hydrogen bond formation.

Borisenko, K.B., Hargittai, I.: J. Mol. Struct. **382** (1996) 171.

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