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(E)-3-[(3-(Trifluoromethyl)phenylimino) methyl] benzene-1,2-diol: X-ray and DFT calculated structures

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Abstract: The crystal structure of (E)-3-[(3-(Trifluoromethyl)phenylimino)- methyl] benzene-1,2-diol was determined using X-ray diffraction and the molecular structure was investigated with density functional theory (DFT). The X-ray study showed that the title compound has a strong intramolecular O-H...N hydrogen bond and 3-dimensional crystal networks are primarily determined by O-H...O intermolecular hydrogen bonds and weak van der Waals interactions. The strong O-H...N bond is evidence of the preference for the phenol-imine tautomeric form in the solid state.