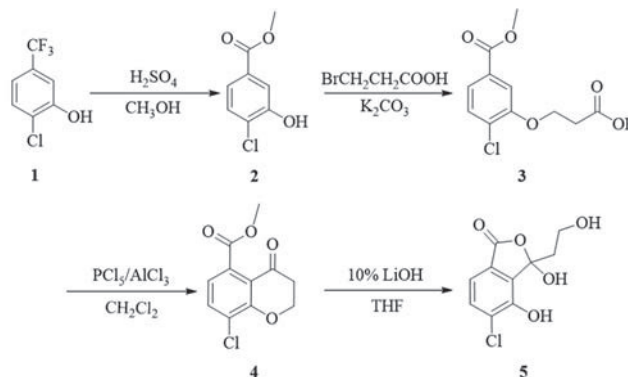


Synthesis and Crystal Structure of 5-Chloro-3,4-dihydroxy-3-(2-hydroxyethyl)isobenzofuran-1(3*H*)-one

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ABSTRACT 5-Chloro-3,4-dihydroxy-3-(2-hydroxyethyl)isobenzofuran-1(3*H*)-one ($C_{10}H_9ClO_5$, $M_r=244.63$) has been synthesized using 2-chloro-5-trifluoromethylphenol as starting material through esterification, Friedel-Crafts acylation, hydrolysis, and cyclization reaction. The compound was characterized by infrared (IR), 1H nuclear magnetic resonance (NMR), ^{13}C NMR, and elemental analysis. The single crystal structure of the title compounds has been further determined by X-ray diffraction. The crystal belongs to the triclinic system, space group $P\bar{1}$ with $a=7.8111(16)$ Å, $b=7.8164(16)$ Å, $c=8.5660(17)$ Å, $\alpha=82.50(3)^\circ$, $\beta=71.28(3)^\circ$, $\gamma=68.22(3)^\circ$, $V=459.93(16)$ Å³, $Z=2$, $D_c=1.766$ g/cm³, $\mu=0.418$ mm⁻¹, $F(000)=252$, the final $R_1=0.0792$, and $wR_2(I>2\sigma(I))=0.2209$. The existence of π - π conjunction effect resulted in correlative bond length shorter than typical bond length in the crystal. The title compound is assembled into a three-dimensional supramolecular structure by two intermolecular hydrogen bonds and one intramolecular hydrogen bond.



KEYWORDS 5-Chloro-3,4-dihydroxy-3-(2-hydroxyethyl)isobenzofuran-1(3*H*)-one, Synthesis, Single crystal structure.