
Crystal structure of (Z)-5-(4-chlorobenzylidene)-2-thioxothiazolidin-4-one —dimethylsulfoxide (1:1), $C_{12}H_{12}ClNO_{2}S_{3}$

Abstract

$C_{12}H_{12}ClNO_{2}S_{3}$, triclinic, $P\bar{1}$ (no. 2), $a = 4.4065(7)$ Å, $b = 12.326(2)$ Å, $c = 13.399(2)$ Å, $\beta = 96.032(6)^{\circ}$, $V = 718.2(2)$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.0668$, $wR(F^2) = 0.164$, $T = 100$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The chemical reagents and solvents used in this study are commercially available. The synthesis of (Z)-5-(4-chlorobenzylidene)-2-thioxothiazolidin-4-one follows a reported synthesis [1]. The product was recrystallized from DMSO. All data are matching with reported procedures [1].
The 2-thioxothiazolidin-4-one (Rhodanine) skeleton represents the key pharmacophore of several pharmaceutically agents. Thus, several substituted 2-thioxothiazolidin-4-one for example pioglitazone (hypoglycemic), etozoline (antihypertensive), thiazolidomycin (activity against Strep- tomyces species), and ralitoline (anticonvulsant), based on this pharmacophore are already in the market. On the other hand, this scaffold shows antifungal, antibacterial, antiviral, anti-inflammatory, anticonvulsant, anti-diabetic, anti-proliferative, anti-tubercular, anti-hyperlipidemic, and antiviral, anti-inflammation, anticonvulsant, anti-diabetic, other hand, this scaffold shows antifungal, antibacterial, antiviral, anti-inflammatory, anticonvulsant, anti-diabetic, anti-proliferative, anti-tubercular, anti-hyperlipidemic, and cardiovascular activities. In continues of our research [2, 3] we report the crystal structure of a new thioxothiazolidin-4-one compound [4–6]. The title compound, C3. The dihedral angle between the two rings is 5.79(2). A chlorobenzylidene moiety is connected to C3. The dihedral angle between the two rings is 5.79(2). The asymmetric unit involves a dimethylsulfoxide (DMSO) solvate molecules which plays a crucial role in the stabilization of the molecular crystal structure because of its NH···O hydrogen bond.

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References


