

Crystal Structure of 7-methyl [3-(2-(4-Chlorophenyl sulfonyl) ethenyl]-4H-1-Benzopyran-4-one

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Abstract

Sulfones display activity as antibacterial and antifungal agents. Dapsone has been proven to be effective against leprosy and diasone is found to be highly effective against streptococci and pneumococci infections. The antifungicidal activity of some unsaturated sulfones has been found to be dependent upon substituent and stereochemical effect. In the title compound $C_{17}H_{14}ClO_4S$, contains three nearly planar segments (the benzopyranone group, the chlorophenyl ring and the ethene group). The sulfonyl plane is inclined at $52.8(2)$ degrees to the plane of the chlorophenyl group and at $48.9(2)$ degrees to the plane of the benzopyranone group. Crystals obtained from 2 propanal by slow evaporation are monoclinic, $a=12.91(7)$, $b=9.708(6)$ and $c=14.372(4)$ Å, $\beta=112.54(2)$ degrees; $V=1655.1(3)$ Å³, $M_w=360.81$, $\lambda(\text{MoK}\alpha)=0.71073$ Å. The structure was solved by direct methods and refined by full matrix least squares using SHELXL-97 to final values of $R=0.0791$ and $R_w=0.2703$ for 2794 symmetry independent reflections collected using Bruker Smart diffractometer.

KEYWORD: x-ray structure , benzopyranone group.

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