

2-Methoxy-4-[(5-oxo-2-phenyl-4,5-dihydro-1,3-oxazol-4-ylidene)methyl]-phenyl 4-methylbenzenesulfonate

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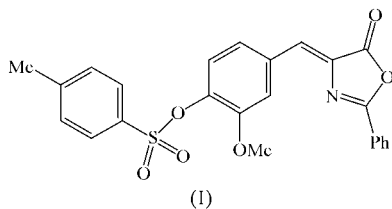
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Molecules of the title compound, C₂₄H₁₉NO₆S, adopt the *Z* configuration and have a distorted tetrahedral geometry around the S atom. The oxazolone, 2-phenyl and methoxyphenyl rings are approximately coplanar. The C atom between the methoxyphenyl and oxazolone rings displays a distorted trigonal bonding geometry. Pairs of molecules are linked into dimers through weak C—H···O hydrogen bonds.

Comment

Oxazolones are a class of small heterocycles which are important intermediates for the synthesis of several molecules, such as amino acids, peptides, antimicrobial and antitumour compounds, heterocyclic precursors, and biosensors and photosensitive devices for proteins. Some oxazolones have shown a wide range of pharmaceutical properties (Mesaik *et al.*, 2004; Paul *et al.*, 2004; Beccalli *et al.*, 1999; Avenozza *et al.*, 2002). Extensive studies on oxazolone dyes have shown favourable photophysical and photochemical properties in the crystalline state, which has resulted in their use in semiconductor devices, such as electrophotographic photo-receptors, and in non-linear optical materials (Ertekin *et al.*, 2003).



In the title compound, (I) (Fig. 1), the N1=C18, C18—O5 and C17=O6 bonds in the oxazolone ring (Table 1) are slightly longer than the corresponding bonds in 4-(4-acetoxybenzylidene)-2-methyl-5-oxazolone [1.279 (3), 1.381 (3) and 1.193 (3) Å, respectively; Haasbroek *et al.*, 2003]. The

O5—C17, C17—C16 and C16—N1 bonds are similar to the corresponding bond lengths in 4-(4-acetoxybenzylidene)-2-methyl-5-oxazolone [1.387 (3), 1.474 (3) and 1.404 (3) Å, respectively; Haasbroek *et al.*, 2003]. All four rings in the molecule of the title compound are essentially planar, the maximum deviation being 0.008 (4) Å for atom C5. The oxazolone ring is approximately coplanar with the 2-phenyl and methoxyphenyl rings [dihedral angles = 6.41 (2) and 7.6 (2)°, respectively], but is twisted with respect to the 4-methylphenyl ring [dihedral angle = 57.93 (10)°].

The molecule adopts the *Z* configuration, and the coplanarity and conjugation of the π -electron systems in the aromatic rings are reflected in the C—C bond lengths between the oxazolone and methoxyphenyl rings. The C15—C16 bond is significantly shorter than the C11—C15 bond. Because of

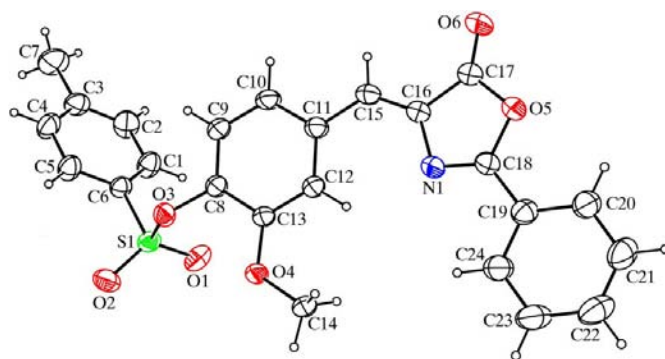


Figure 1

An ORTEP (Burnett & Johnson, 1996) view of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary size.

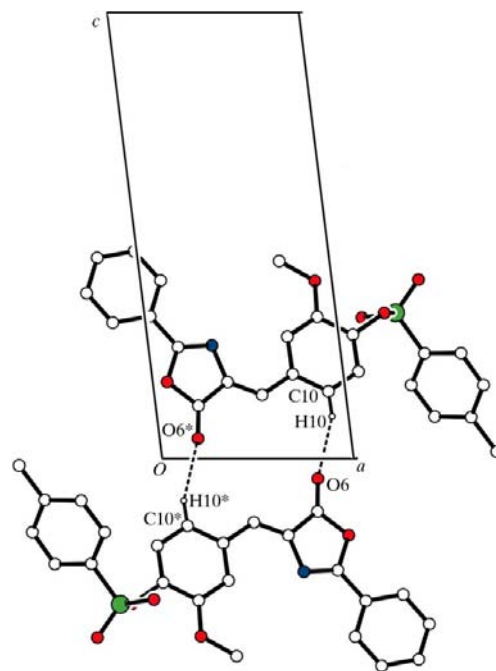


Figure 2

The crystal packing of (I), showing the weak interaction, doubled by the crystallographic inversion centre, stabilizing the dimers (dashed lines). Atoms marked with an asterisk (*) are generated through inversion (symmetry code: $-x + 1, -y, -z$).

the steric hindrance of the oxazolone and aromatic rings, atom C15 has a distorted trigonal geometry, with the angle deviating significantly from the ideal trigonal value, as found also in previously reported analogues (Delgado *et al.*, 2005, 2006). The S atom has a distorted tetrahedral geometry.

The crystal structure of (I) is determined by rather weak C—H...O interactions (Desiraju & Steiner, 1999). Inter-molecular C—H...O hydrogen bonding (Table 2 and Fig. 2) consists of centrosymmetric dimer units containing a 14-membered ring (Aygün *et al.*, 1988).

Experimental

A solution of 3-methoxy-4-(4-methylphenylsulfonyloxy)benzaldehyde (1.0 g, 3 mmol), benzoylglycine (0.54 g, 3 mmol), acetic anhydride (0.6 ml, 6 mmol) and sodium acetate (0.41 g, 3 mmol) was heated until the mixture just liquified, and then heating was continued for a further 2 h. After the completion of the reaction (determined by thin-layer chromatography), ethanol (20 ml) was added and the mixture was kept at room temperature for 18 h. The solid product thus obtained was purified by washing with cold ethanol, hot water and then a small amount of hexane. The solid was recrystallized from hot ethanol and pure orange crystals were obtained.

Crystal data

$C_{24}H_{19}NO_6S$	$\gamma = 99.492 (8)^\circ$
$M_r = 449.46$	$V = 1072.82 (19) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 6.7854 (7) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.2766 (11) \text{ \AA}$	$\mu = 0.19 \text{ mm}^{-1}$
$c = 16.0242 (15) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\alpha = 101.338 (8)^\circ$	$0.48 \times 0.15 \times 0.05 \text{ mm}$
$\beta = 94.775 (8)^\circ$	

Data collection

Stoe IPDSII diffractometer	9923 measured reflections
Absorption correction: integration (<i>XRED32</i> ; Stoe & Cie, 2002)	4206 independent reflections
$T_{\min} = 0.913$, $T_{\max} = 0.990$	2745 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.067$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$	290 parameters
$wR(F^2) = 0.133$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
4206 reflections	$\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

O5—C17	1.387 (3)	N1—C18	1.283 (3)
O5—C18	1.385 (3)	C11—C15	1.457 (4)
O6—C17	1.202 (3)	C15—C16	1.339 (4)
N1—C16	1.400 (3)	C16—C17	1.467 (4)
O1—S1—O2	120.99 (14)	O2—S1—C6	109.30 (12)
O1—S1—O3	109.56 (12)	O3—S1—C6	103.23 (11)
O2—S1—O3	103.03 (12)	C8—O3—S1	119.98 (16)
O1—S1—C6	109.18 (13)	C11—C15—C16	128.3 (2)
C6—S1—O3—C8	−85.14 (18)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C10—H10...O6 ⁱ	0.93	2.52	3.405 (3)	158
C12—H12...N1	0.93	2.31	2.975 (4)	128

Symmetry code: (i) $-x + 1, -y, -z$.

All H atoms were treated as riding atoms, with C—H distances of 0.93–0.96 \AA and with $U_{\text{iso}}(\text{H}) = kU_{\text{eq}}(\text{C})$, where $k = 1.5$ for methyl and $k = 1.2$ for all other H atoms.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD3084). Services for accessing these data are described at the back of the journal.

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