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Supplementary data for this paper are available from the IUCr electronic archives (Reference: KA1286). Services for accessing these data are described at the back of the journal.

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4-Chloro-2-{4-[*p*-(methylsulfonyl)phenyl]-2-oxo-5-phenyl-2,3-dihydro-1,3-oxazol-3-yl}-phenyl Acetate

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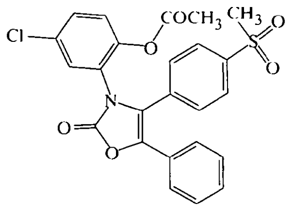
Abstract

In the title triaryloxazolone derivative, $C_{24}H_{18}ClNO_6S$, the three phenyl rings are oriented in a propeller-like fashion around the central oxazolone ring, with dihedral angles of 55.7 (1) (acetoxyphenyl), 56.4 (1) (methylsulfonylphenyl) and 25.0 (1)° (phenyl).

Comment

In the course of investigating the structure–activity relationships of COX-2 (cyclooxygenase II) inhibitors (Thérien *et al.*, 1997), we isolated an unknown product from the condensation reaction of 2-amino-5-chlorobenzoxazole with 2-bromo-2-[4-(methylsulfonyl)-phenyl]-1-phenylethanone. Conversion of this compound to an acetate, (I), permitted crystallization. The subsequent crystal structure determination unequivocally established the connectivity of this compound. Knowing the structure and the results of isotopic labelling studies permitted the proposal of a mechanism for the formation of this triaryloxazolone derivative (Roy *et al.*, 1997).



(I)

The conformation adopted by the molecule is shown in Fig. 1, which also shows the crystallographic numbering scheme. The dihedral angles between the oxazolone ring and the substituent phenyl rings are: 55.7 (1)° with ring C2–C7, 25.0 (1)° with ring C13–C18 and 56.4 (1)° with ring C19–C24. All bond distances and angles agree well with values for similar types of bonds reported in the Cambridge Structural Database (Allen & Kennard, 1993).

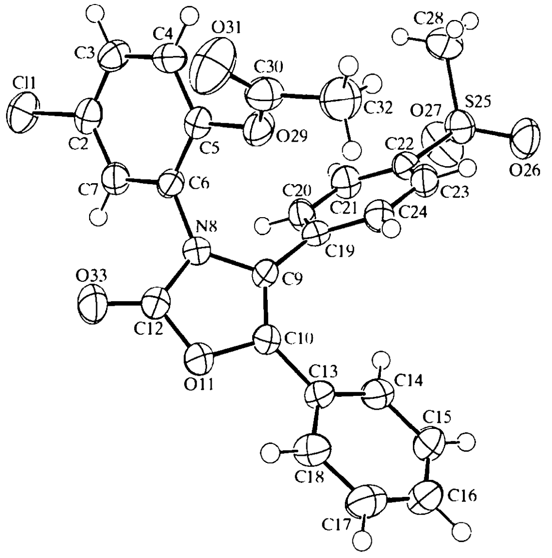


Fig. 1. The molecular conformation of (I) showing the crystallographic numbering scheme. Ellipsoids are drawn at the 50% probability level, while H atoms are represented by circles of arbitrary size.

Examination of the packing in the unit cell shows that the molecules pack as discrete monomeric units. An analysis of C—H···O interactions yielded none worthy of note. Similarly, no significant ring–ring interactions were observed with neighbouring molecules.

Experimental

The title compound was synthesized as described previously (Roy *et al.*, 1997) and single crystals suitable for diffraction measurements were obtained from methanol/water.

Crystal data

$C_{24}H_{18}ClNO_6S$
$M_r = 483.931$
Monoclinic
$P2_1/n$
$a = 10.4968\,(9)$ Å
$b = 13.500\,(1)$ Å
$c = 15.626\,(1)$ Å
$\beta = 96.986\,(6)°$
$V = 2197.9\,(6)$ Å^3
$Z = 4$
$D_x = 1.462$ Mg m^{-3}
D_m not measured
Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 24 reflections
$\theta = 37.09–39.89°$
$\mu = 2.79$ mm^{-1}
$T = 294$ K
Small rhomb
0.12 × 0.12 × 0.12 mm
Colourless

Data collection

Rigaku AFC-5 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
4700 measured reflections
4253 independent reflections
3033 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\rm max} = 72.65°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 16$
$l = -19 \rightarrow 19$
3 standard reflections every 400 reflections intensity decay: −1.0 (4)%

Refinement

Refinement on F^2
$R(F) = 0.049$
$wR(F^2) = 0.128$
$S = 1.026$
4253 reflections
300 parameters
H atoms riding
$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.8774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = -0.001$
$\Delta\rho_{\rm max} = 0.51\,(7)$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.32\,(7)$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected bond lengths (Å)*

Cl1—C2	1.741 (3)	N8—C9	1.406 (3)
O11—C12	1.353 (4)	N8—C6	1.427 (3)
O11—C10	1.400 (3)	C9—C10	1.337 (4)
O33—C12	1.209 (4)	C9—C19	1.474 (4)
N8—C12	1.369 (4)	C10—C13	1.463 (4)

H atoms were included at calculated positions using a riding model (with this model each methyl group contributes an additional parameter to those varied).

Data collection: AFC-5 software. Cell refinement: AFC-5 software. Data reduction: local software. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP* (Johnson, 1965). Software used to prepare material for publication: local software.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1376). Services for accessing these data are described at the back of the journal.

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Methyl 2,6-Dihydroxy-4-(2-hydroxy-4,6-dimethoxy-3-methylbenzoyloxy)-3-methylbenzoate

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Abstract

In the title compound, $C_{19}H_{20}O_9$, the benzene rings are nearly perpendicular to each other [dihedral angle 86.39 (8)°]. All three hydroxy groups are involved in intramolecular O—H···O hydrogen bonds.

Comment

The biosynthetic interrelationship between the common depsides, the depsidones, dibenzofurans and diphenyl ethers has been a subject of speculation for some time (Culberson, 1969; Mosbach, 1973). It has been reported

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