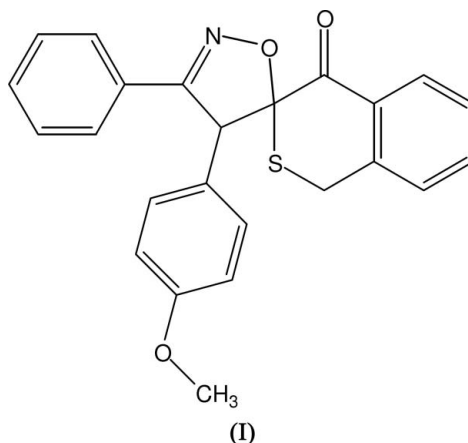


4'-(4-Methoxyphenyl)-3'-phenylspiro[1*H*-isothia-
chroman-3,5'-isoxazolidin]-4(2*H*)-oneBennani Brahim,^a Kerbal
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Key indicators

Single-crystal X-ray study
 $T = 173\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.030
 wR factor = 0.075
Data-to-parameter ratio = 15.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The crystal structure determination of the new title spiro-
isoxazoline, $\text{C}_{24}\text{H}_{19}\text{NO}_3\text{S}$, shows that the five-membered
isoxazoline ring is coplanar with the phenyl ring attached to
it. The *p*-methoxyphenyl ring is almost perpendicular to the
isoxazoline ring.

Comment

Spiroisoxazolines display interesting biological properties,
such as herbicidal, plant-growth regulatory and antitumour
activities (Howe & Shelton, 1990; Smietana *et al.*, 1999). Many
4-chromanone derivatives are versatile intermediates for the
synthesis of natural products such as brazillin, hematoxylin,
ripariochromene, clausenin, calonlide A and inophyllum B
(Kooijman *et al.*, 1984; Chenera *et al.*, 1993). Chromanone
heterocycles have also attracted much attention owing to their
important pharmacological properties (Chaouni-Benabdallah
et al., 2001). Their high synthetic utility and pharmacological
importance have prompted us to synthesize some biologically
active spiroisoxazoline derivatives, one of which is the title
compound, (I).A perspective view of (I) is shown in Fig. 1. Bond lengths
and angles can be regarded as normal (Cambridge Structural
Database, Version 5.27 plus one update; *MOGUL* Version 1.1;
Allen, 2002). The essentially planar (r.m.s. deviation =
0.101 Å) isoxazolidine ring is almost coplanar with the phenyl
ring attached to it. The dihedral angle between the two rings is
4.71 (9)°. The *p*-methoxyphenyl ring, on the other hand,
encloses a dihedral angle of 80.04 (4)° with the isoxazolidine
ring. The S-containing heterocycle adopts a half-chair
conformation, with atoms C1, C11, C12 and C3 in a common
plane and atoms C2 and S1 deviating by 0.424 (3) and
−0.524 (3) Å, respectively, from this plane.

The present study shows that the conformation of (I) is in agreement with the results reported previously (Katritzky *et al.*, 2003, Bakavoli *et al.*, 2005).

Experimental

To a solution (10 ml) of 3-arylideneisothiochroman-4-one and *N*-benzhydroxyiminoyl chloride in dry chloroform, sodium hypochlorite (10 mmol) was added. The reaction mixture was stirred at low temperature (from 263–268 K) until the disappearance of the starting materials, as monitored by thin-layer chromatography, was observed. When the reaction was complete, the solution was filtered and the solvent was removed *in vacuo*. The resulting crude product was purified by column chromatography to obtain a high yield. Crystals of (I) were grown by slow evaporation of an ethanol solution.

Crystal data

C ₂₄ H ₁₉ NO ₃ S	$D_x = 1.375 \text{ Mg m}^{-3}$
$M_r = 401.46$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 19447 reflections
$a = 5.9564 (5) \text{ \AA}$	$\theta = 2.2\text{--}26.4^\circ$
$b = 26.2779 (19) \text{ \AA}$	$\mu = 0.19 \text{ mm}^{-1}$
$c = 12.4460 (9) \text{ \AA}$	$T = 173 (2) \text{ K}$
$\beta = 95.553 (6)^\circ$	Block, colourless
$V = 1938.9 (3) \text{ \AA}^3$	$0.45 \times 0.42 \times 0.32 \text{ mm}$
$Z = 4$	

Data collection

Stoe IPDS-II two-circle diffractometer	4015 independent reflections
ω scans	3122 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$R_{\text{int}} = 0.055$
$T_{\text{min}} = 0.920$, $T_{\text{max}} = 0.940$	$\theta_{\text{max}} = 26.6^\circ$
25474 measured reflections	$h = -7 \rightarrow 7$
	$k = -32 \rightarrow 32$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.030$	$w = 1/[\sigma^2(F_o^2) + (0.044P)^2]$
$wR(F^2) = 0.075$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4015 reflections	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
263 parameters	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$

Table 1

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

C1–S1	1.8051 (13)	N1–C5	1.2857 (16)
S1–C2	1.7965 (12)	N1–O1	1.4307 (13)
C2–S1–C1	98.22 (6)	N1–O1–C2	107.75 (8)
O1–C2–C4	104.84 (9)	C5–C4–C2	98.84 (9)
C5–N1–O1	108.83 (10)	N1–C5–C4	114.38 (11)

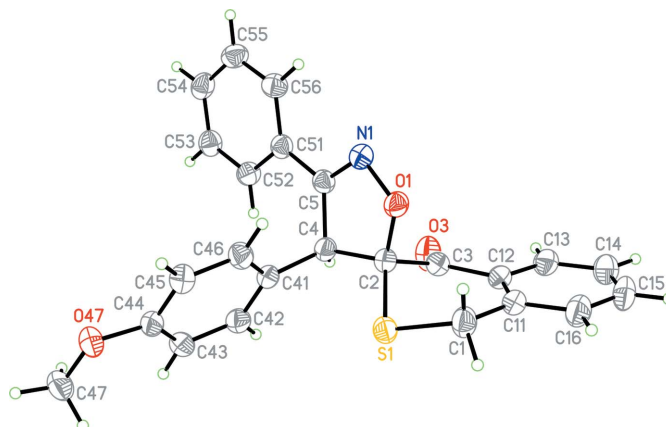


Figure 1

A perspective view of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

All H atoms were located in a difference map, but were refined with fixed individual displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$] using a riding model, with C–H = 0.95–1.00 \AA . The methyl group was allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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