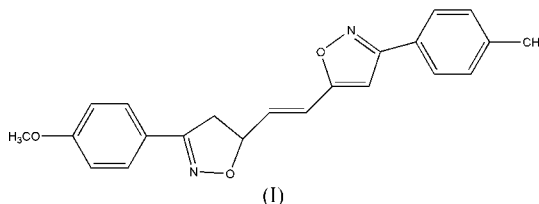


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Key indicators

Single-crystal X-ray study
T = 296 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.048
wR factor = 0.113
Data-to-parameter ratio = 6.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.5-{2-[3-(4-Methoxyphenyl)-4,5-dihydroisoxazol-5-yl]vinyl}-3-*p*-tolylisoxazoleThe title compound, $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}_3$, displays a *trans* configuration with respect to the olefinic link. The isoxazole and benzene rings are slightly twisted towards each other.

Comment

Isoxazole and isoxazoline moieties represent two classes of unique pharmacophores that are observed in many therapeutic agents and are versatile intermediates for the synthesis of complex natural products. Therefore, they are interesting targets in the development of new drug leads. In the title compound, (I), the fact that the C19–O3–C22 angle is $116.9(2)^\circ$ shows the influence of the benzene ring on the ether group. The widening of the C5–C8–C9 [to $130.1(3)^\circ$] and C9–C10–C11 [to $133.9(3)^\circ$] angles, and the decrease in the C13–C14–C15 and O2–C13–C14 angles [$101.6(2)$ and $104.0(2)^\circ$, respectively], may be due to steric effects. The olefinic bond of the title compound exhibits a *trans* configuration. The dihedral angles between the isoxazoline plane and the two benzene planes are $75.14(4)$ and $171.55(2)^\circ$, and the dihedral between the two benzene rings is $97.85(3)^\circ$.

Experimental

Phenylpropargyl selenide (2 mmol) was mixed with hydroximoyl halide (2 mmol); to the mixture was added Et_3N , dropwise for 6 h, yielding 3-(4-methylphenyl)-5-phenylselenomethylisoxazole, which react with lithium diisopropylamide and allyl bromide, followed by another 1,3-dipolar cycloaddition (Kurth & Kantorowski, 1997) to obtain isoxazolyl and isoxazolyl substituted [viz. (I)] olefins were obtained through selenoxide *syn* elimination of selenide (Clive, 1978). The solid was filtered off and single crystals suitable for X-ray analysis were obtained by recrystallization from chloroform.

Crystal data

 $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}_3$
 $M_r = 360.41$
Orthorhombic, $Pca2_1$
 $a = 9.9819(2) \text{ \AA}$
 $b = 22.3639(4) \text{ \AA}$
 $c = 8.4150(1) \text{ \AA}$
 $V = 1878.52(6) \text{ \AA}^3$
 $Z = 4$
 $D_x = 1.274 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation
Cell parameters from 18 400 reflections
 $\theta = 2.2\text{--}27.4^\circ$
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 296(1) \text{ K}$
Platelet, yellow
 $0.45 \times 0.34 \times 0.10 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID
diffractometer
 ω scans
15 501 measured reflections
2283 independent reflections
1257 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.032$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -12 \rightarrow 12$
 $k = -29 \rightarrow 29$
 $l = -9 \rightarrow 10$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.113$
 $S = 1.01$
1637 reflections
244 parameters

H-atom parameters constrained
 $w = 1/[0.001F_o^2 + 0.76\sigma^2(F_o)]/(4F_o^2)$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.34 \text{ e } \text{\AA}^{-3}$

Table 1

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

O1—N1	1.412 (3)	C6—C7	1.386 (5)
O1—C10	1.346 (3)	C8—C9	1.403 (4)
O2—N2	1.416 (3)	C9—C10	1.345 (4)
O2—C13	1.453 (3)	C10—C11	1.450 (4)
O3—C19	1.366 (3)	C11—C12	1.321 (4)
O3—C22	1.433 (4)	C12—C13	1.478 (4)
N1—C8	1.315 (4)	C13—C14	1.530 (4)
N2—C15	1.275 (3)	C14—C15	1.493 (4)
C1—C2	1.514 (4)	C15—C16	1.463 (4)
C2—C3	1.379 (5)	C16—C17	1.400 (4)
C2—C7	1.365 (5)	C16—C21	1.388 (4)
C3—C4	1.382 (4)	C17—C18	1.372 (4)
C4—C5	1.379 (4)	C18—C19	1.384 (4)
C5—C6	1.392 (4)	C19—C20	1.370 (4)
C5—C8	1.472 (4)	C20—C21	1.384 (4)
C19—O3—C22	116.9 (2)	C9—C10—C11	133.9 (3)
C3—C2—C7	117.2 (3)	O2—C13—C14	104.0 (2)
C4—C5—C6	117.6 (3)	C13—C14—C15	101.6 (2)
C5—C8—C9	130.1 (3)	C17—C16—C21	117.5 (3)

H atoms were placed in calculated positions, with C—H = 1.00 \AA , and included in the final cycles of refinement in a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

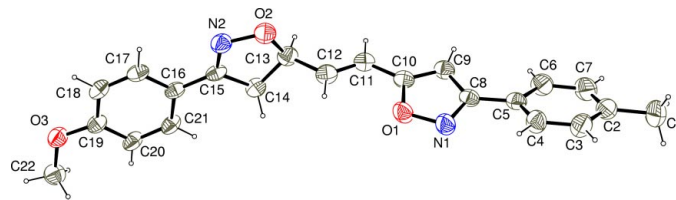


Figure 1

Molecular structure of the title compound, with 30% probability displacement ellipsoids.

Data collection: *PROCESS-AUTO* (Rigaku/MSC & Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku Corporation, 2001); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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