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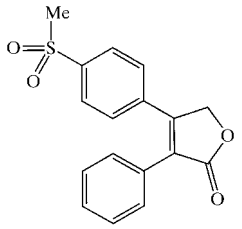
Viox {2,5-dihydro-4-[4-(methylsulfonyl)phenyl]-3-phenyl-2-furanone, $C_{17}H_{14}O_4S$, (I)} is one of the selective COX-II inhibitors with anti-arthritic activity. The absolute structure of viox has been determined on the basis of anomalous scattering effects. Molecules are held together in the crystal structure only by normal van der Waals interactions.



(I)

Experimental

Crystals suitable for diffraction analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{17}H_{14}O_4S$
M_r = 314.36
Tetragonal, $P4_12_12$
a = 11.374 (2) Å
c = 22.939 (3) Å
V = 2967.6 (9) Å^3
Z = 8
D_x = 1.407 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 21.1–29.1°
μ = 2.082 mm^{-1}
T = 298.2 K
Block, yellow
0.50 × 0.50 × 0.30 mm

Data collection

Rigaku AFC-7*S* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.390, T_{max} = 0.535
1682 measured reflections
1682 independent reflections
1656 reflections with $I > 0$
θ_{max} = 70.07°
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 26$
3 standard reflections
every 150 reflections
intensity decay: 0.41%

Refinement

Refinement on F
R = 0.042
wR = 0.059
S = 1.740
1656 reflections
200 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o) + 0.00063|F_o|^2]$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: Zachariasen (1967)
Extinction coefficient: 1.22 (9) × 10^{-5}

Table 1
Selected geometric parameters (Å, °).

S(1)—O(3)	1.433 (2)	O(1)—C(8)	1.350 (5)
S(1)—O(4)	1.436 (2)	O(1)—C(9)	1.434 (4)
S(1)—C(14)	1.756 (3)	O(2)—C(8)	1.202 (4)
S(1)—C(17)	1.749 (3)		
O(3)—S(1)—O(4)	118.5 (1)	O(1)—C(8)—O(2)	122.0 (3)
O(3)—S(1)—C(14)	108.3 (1)	O(1)—C(8)—C(7)	109.2 (3)
O(3)—S(1)—C(17)	108.1 (1)	O(2)—C(8)—C(7)	128.8 (4)
O(4)—S(1)—C(14)	108.1 (1)	O(1)—C(9)—C(10)	105.2 (3)
O(4)—S(1)—C(17)	109.0 (1)	S(1)—C(14)—C(13)	118.8 (2)
C(14)—S(1)—C(17)	103.9 (1)	S(1)—C(14)—C(15)	120.7 (2)
C(8)—O(1)—C(9)	109.1 (2)		

The absolute structure was determined by refining the reported structure and the inverted form in space group $P4_32_12$; the alternative model gave R = 0.0512, wR = 0.0726, S = 2.14 for the same number of data and parameters, and so can be rejected as incorrect.

Data collection: *MSC/AFC Diffractometer Control Software* (MSC, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *teXsan* (MSC, 1992–1997); program(s) used to refine structure: *teXsan* (MSC, 1992–1997); software used to prepare material for publication: *teXsan* (MSC, 1992–1997).

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