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Methyl 2-{[3-(4-methylsulfanyl)phenyl-1,2,4-oxadiazol-5-yl]methoxy}phenylacetate

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Key indicators

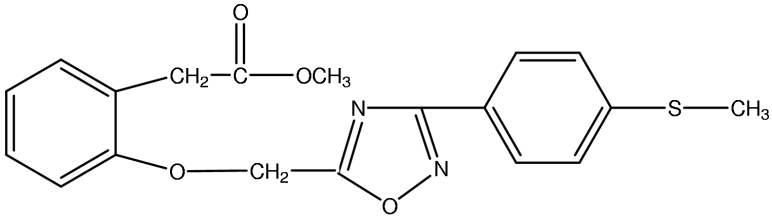
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.142
Data-to-parameter ratio = 14.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{19}H_{18}N_2O_4S$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and 3-(4-methylthio)phenyl-5-chloromethyl-1,2,4-oxadiazole. The structure exhibits intermolecular C—H···O hydrogen bonds and C—H···π interactions.

Comment

1,2,4-Oxadiazole derivatives are of great interest because of their biological properties. Some derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties and show high efficacy as agonists [*e.g.* for muscarinic (Macor *et al.*, 1996), adrenergic (Quagliato & Andrae, 2002) and 5-hydroxytryptamine (Gur *et al.*, 2001)] and antagonists [*e.g.* for angiotensin (Naka & Kubo, 1999) and adhesion (Juraszyk *et al.*, 1997)] for different receptors. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1 and bond lengths, angles and torsion angles are given in Table 1. In the crystal structure, molecules are linked by C—H···O hydrogen bonds (Table 2). There are also C—H···π interactions in the crystal structure (Table 2 and Fig. 3).

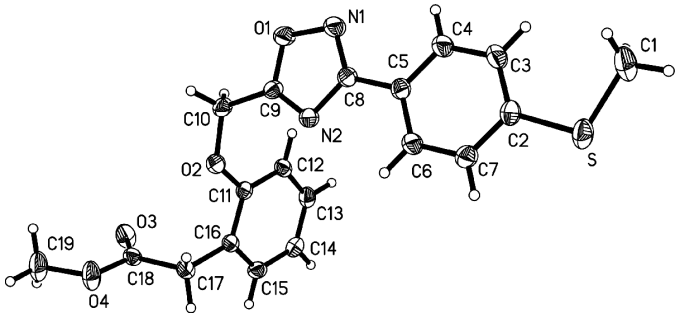


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

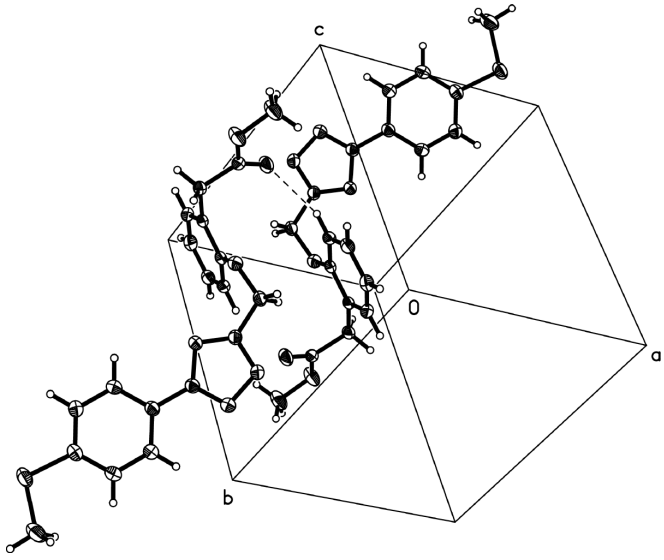


Figure 2
The short C—H···O contact (dashed line) in the crystal structure of (I).

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolved in acetone (20 ml) and potassium carbonate (30 mmol) was added in one portion. 3-[(4-Methylsulfanyl)phenyl]-5-chloromethyl-1,2,4-oxadiazole (20 mmol) in acetone (20 ml) was added to this mixture. The resulting mixture was refluxed for 6 h, then concentrateed under reduced pressure to afford crude compound (I). Pure compound (I) was obtained by crystallization from ethyl acetate (m.p. 359–360 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$): δ 7.98–8.00 (*m*, 2H), 7.31–7.32 (*m*, 2H), 7.23–7.27 (*m*, 2H), 6.98–7.03 (*m*, 2H), 5.34 (*s*, 2H), 3.73 (*s*, 2H), 3.69 (*s*, 3H), 3.52 (*s*, 3H).

Crystal data

$C_{19}H_{18}N_2O_4S$
M_r = 370.41
Triclinic, $P\overline{1}$
a = 8.3580 (17) Å
b = 10.522 (2) Å
c = 10.581 (2) Å
α = 90.13 (3)°
β = 102.08 (3)°
γ = 99.73 (3)°
V = 896.1 (3) Å^3
Z = 2
D_x = 1.373 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–13°
μ = 0.21 mm^{-1}
T = 293 (2) K
Block, colourless
0.4 × 0.3 × 0.3 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3752 measured reflections
3499 independent reflections
2763 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.0°
$h = 0 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 12$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.142
S = 0.91
3499 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.35P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.014
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.036 (5)

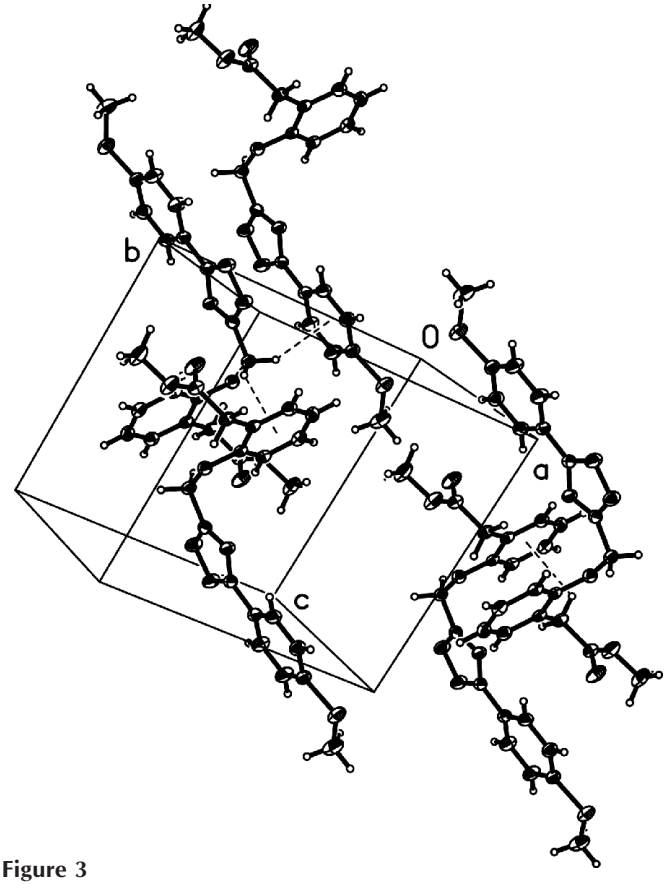


Figure 3
The C—H···π interactions in (I), shown as dashed lines.

Table 1
Selected geometric parameters (Å, °).

S—C2	1.757 (2)	O4—C19	1.442 (3)
S—C1	1.782 (3)	N1—C8	1.304 (3)
O1—C9	1.334 (2)	N2—C8	1.380 (2)
O1—N1	1.416 (2)	N2—C9	1.292 (2)
O2—C10	1.415 (2)	C5—C8	1.468 (3)
O2—C11	1.378 (2)	C9—C10	1.496 (3)
O3—C18	1.200 (2)	C16—C17	1.505 (3)
O4—C18	1.339 (2)	C17—C18	1.504 (2)
C2—S—C1	104.11 (12)	N2—C9—C10	130.83 (18)
C9—O1—N1	106.07 (14)	O1—C9—C10	115.29 (16)
C11—O2—C10	118.04 (15)	O2—C10—C9	113.34 (15)
C18—O4—C19	115.95 (17)	O2—C11—C12	123.99 (17)
C8—N1—O1	103.23 (16)	O2—C11—C16	115.13 (16)
C9—N2—C8	102.45 (16)	C15—C16—C17	120.89 (17)
C7—C2—S	117.43 (17)	C11—C16—C17	120.87 (17)
C4—C5—C8	120.43 (18)	C18—C17—C16	113.25 (15)
N1—C8—N2	114.38 (17)	O3—C18—O4	122.65 (18)
N1—C8—C5	122.09 (18)	O3—C18—C17	126.41 (18)
N2—C8—C5	123.50 (17)	O4—C18—C17	110.87 (16)
N2—C9—O1	113.87 (17)		
C9—O1—N1—C8	0.2 (2)	C9—N2—C8—N1	0.4 (2)
N1—O1—C9—C10	178.57 (17)	C9—N2—C8—C5	−177.86 (18)
N1—O1—C9—N2	0.1 (2)	C8—N2—C9—O1	−0.3 (2)
C11—O2—C10—C9	−80.0 (2)	C8—N2—C9—C10	−178.5 (2)
C10—O2—C11—C16	−171.15 (17)	C6—C5—C8—N2	−8.0 (3)
C10—O2—C11—C12	9.2 (3)	C4—C5—C8—N2	170.72 (19)
C19—O4—C18—C17	−179.3 (2)	C6—C5—C8—N1	173.9 (2)
C19—O4—C18—O3	−2.3 (3)	C4—C5—C8—N1	−7.4 (3)
O1—N1—C8—C5	177.94 (17)	N2—C9—C10—O2	−8.8 (3)
O1—N1—C8—N2	−0.3 (2)	O1—C9—C10—O2	173.01 (17)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···O3^{i}	0.93	2.43	3.257 (3)	148
C10—H10A···$Cg2^{ii}$	0.97	2.77	3.58	142
C10—H10B···$Cg3^{i}$	0.97	2.65	3.43	138
C17—H17B···$Cg3^{iii}$	0.97	2.85	3.42	118

Symmetry codes: (i) $2-x,-1-y,3-z$; (ii) $1-x,-1-y,2-z$; (iii) $1-x,-1-y,3-z$. Notes: $Cg2$ is the centroid of atoms C2–C7 and $Cg3$ is the centroid of atoms C11–C16.

All H atoms were bonded to the C atoms were placed geometrically, with C—H = 0.93–0.97 Å, and included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2 or 1.5U_{eq} of the carrier atom.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

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