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5-Chloromethyl-3-[4-(methylsulfonyl)phenyl]-1,2,4-oxadiazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.149
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.

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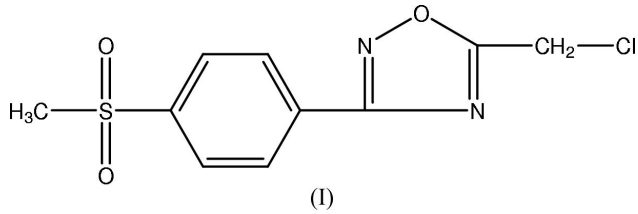
In the crystal structure of the title compound, $C_{10}H_9ClN_2O_3S$, there are intramolecular C—H···O and C—H···N and intermolecular C—H···O hydrogen bonds.

Comment

1,2,4–Oxadiazoles represent an important class of five-membered heterocycles. 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 are efficient as agonists [*e.g.* as angiotension (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, where the dashed lines indicate intramolecular C—H···O and C—H···N hydrogen bonds (Table 2). There are also intermolecular C—H···O hydrogen bonds (Fig. 2). The combination of weak C—H···O interactions generates a three-dimensional network.

Experimental

A solution of chloroacetyl chloride (14 mmol) in toluene (10 ml) was added dropwise to a solution of 4-(methylsulfonyl)benzamidoxime (14 mmol) in toluene (60 ml). The resulting mixture was refluxed for 6 h. After cooling and filtration, crude (I) was obtained. The compound was purified by crystallization from a mixture of ethyl acetate (15 ml) and petroleum ether (7.5 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$): δ 8.29–8.31 (*m*, 2H), 8.07–8.09 (*m*, 2H), 4.78 (*s*, 2H), 3.09–3.10 (*s*, 3H).

Crystal data

$C_{10}H_9ClN_2O_3S$
M_r = 272.70
Monoclinic, $P2_1/c$
a = 5.6170 (11) Å
b = 12.247 (2) Å
c = 16.993 (3) Å
β = 93.06 (3)°
V = 1167.3 (4) Å^3
Z = 4
D_x = 1.552 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–13°
μ = 0.50 mm^{-1}
T = 293 (2) K
Block, colourless
0.4 × 0.3 × 0.3 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2514 measured reflections
2277 independent reflections
1707 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.0°$
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 14$
$l = -20 \rightarrow 20$
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.149$
$S = 1.01$
2277 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl—C10	1.755 (3)	O3—N1	1.413 (3)
S—O2	1.433 (2)	N1—C8	1.307 (3)
S—O1	1.440 (2)	N2—C9	1.281 (4)
S—C1	1.750 (3)	N2—C8	1.373 (3)
S—C2	1.766 (3)	C5—C8	1.465 (4)
O3—C9	1.341 (3)	C9—C10	1.478 (4)
O2—S—O1	117.90 (15)	C9—N2—C8	103.0 (2)
O2—S—C1	109.60 (15)	N1—C8—N2	114.4 (3)
O1—S—C1	108.52 (15)	N1—C8—C5	122.5 (2)
O2—S—C2	108.38 (13)	N2—C8—C5	123.0 (2)
O1—S—C2	107.56 (13)	N2—C9—O3	113.5 (2)
C1—S—C2	103.98 (14)	N2—C9—C10	128.5 (3)
C9—O3—N1	106.3 (2)	O3—C9—C10	118.0 (2)
C8—N1—O3	102.8 (2)	C9—C10—Cl	111.7 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1D···O2^{i}	0.96	2.55	3.490 (4)	167
C3—H3A···O2	0.93	2.59	2.949 (3)	104
C6—H6A···N2	0.93	2.55	2.889 (3)	102
C10—H10A···O1^{ii}	0.97	2.44	3.316 (4)	149

Symmetry codes: (i) $1 + x, y, z$; (ii) $2 - x, -y, -z$.

All H atoms bonded to the C atoms were placed geometrically at distances of 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: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

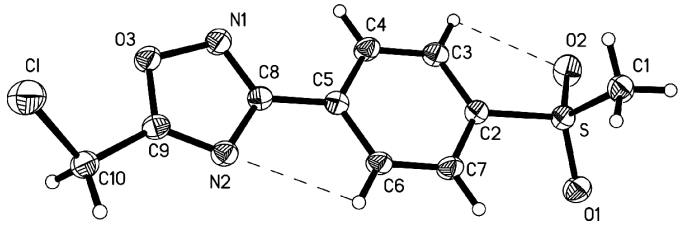


Figure 1
A view of the molecular structure of (I), showing displacement ellipsoids at the 30% probability level. Dashed lines indicate C—H···O and C—H···N hydrogen bonds.

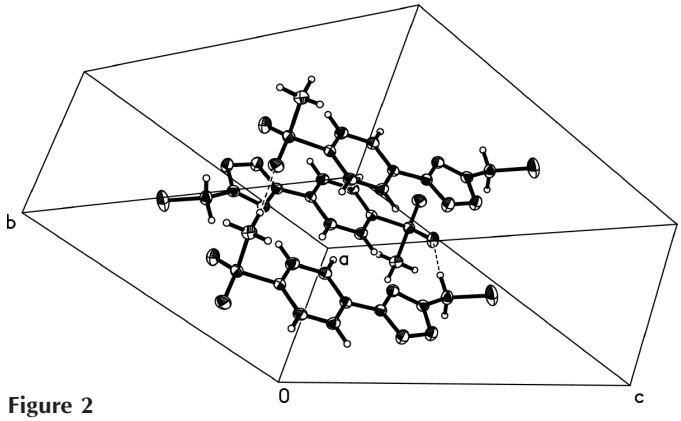


Figure 2
A partial packing diagram of (I). Dashed lines indicate C—H···O hydrogen bonds.

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