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2-Chloro-4-fluorophenyl methanesulfonate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.122
Data-to-parameter ratio = 18.0

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

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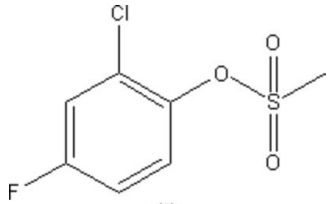
In the crystal structure of the title compound, $C_7H_6ClFO_3S$, molecules form a supramolecular structure *via* intermolecular C—H···O hydrogen bonds and π–π stacking interactions.

Comment

The title compound, (I), is an unexpected product of the reaction of 7-chloro-5-methylsulfanyl-1,2,4-triazolo[1,5-*c*]-pyrimidin-2-yl methanesulfonate with 2-chloro-4-fluoro-phenol.



(I)

The molecular structure of (I) is shown in Fig. 1. Selected bond lengths and angels are shown in Table 1. In the crystal structure, molecules are linked by C—H···O hydrogen bonds (Table 2) to form a chain along the *c* axis (Fig. 2). The packing is further stabilized by π–π stacking interactions between the benzene rings of neighboring molecular chains; the distance between centroids [$Cg\cdots Cg(1-x,1-y,1-z)$] is 3.684 (2) Å and the interplanar spacing is 3.477 (2) Å.

Experimental

A mixture of 2-chloro-4-fluorophenol (4 mmol) and sodium hydride (4 mmol) in anhydrous toluene (60 ml) was stirred at 373 K for 2 h. 7-Chloro-5-methylsulfanyl-1,2,4-triazolo[1,5-*c*]pyrimidin-2-yl methanesulfonate (1 mmol) was then added and the resulting reaction mixture was refluxed for about 2 h. After filtration, the solvent was removed under reduced pressure and the residue was purified by column chromatography on silical gel (eluent: petroleum–acetone 4:1 *v*/*v*) to afford the compound (I) (yield 45%, m.p. 362 K). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.04–7.44 (*m*, 3H, Ar—H), 3.25 (*s*, 3H, CH_3) Crystals suitable for X-ray analysis were grown from a diethyl ethyl ether solution at 277 K.

Crystal data

$C_7H_6ClFO_3S$
M_r = 224.63
Monoclinic, $P2_1/c$
a = 11.2684 (13) Å
b = 7.9014 (9) Å
c = 11.1345 (12) Å
β = 114.284 (2)°
V = 903.65 (18) Å^3
Z = 4
D_x = 1.651 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 1568 reflections
θ = 3.3–21.9°
μ = 0.64 mm^{-1}
T = 292 (2) K
Plate, colorless
0.30 × 0.20 × 0.06 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.832, T_{max} = 0.963
7603 measured reflections
2138 independent reflections
1467 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 28.0°
$h = -14 \rightarrow 14$
$k = -10 \rightarrow 10$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.122
S = 1.04
2138 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.1158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—Cl1	1.720 (3)	O1—S1	1.5996 (18)
C3—F1	1.353 (3)	C7—S1	1.736 (3)
C6—O1	1.407 (3)		
C6—O1—S1	120.05 (15)		
C6—O1—S1—C7	88.1 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O4^{i}	0.96	2.42	3.318 (3)	155

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

H atoms were placed at calculated positions and treated as riding atoms, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(aromatic C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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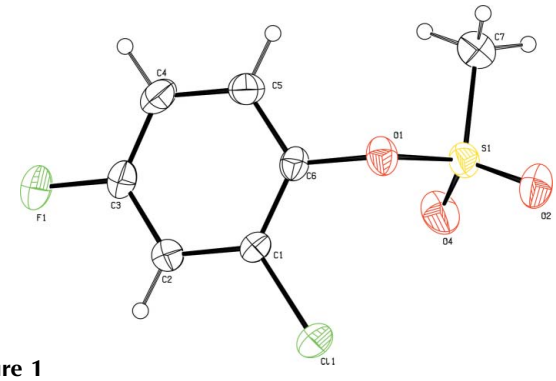

Figure 1
A view of (I), showing the atom-labellng scheme. Displacement ellipsoids are drawn at the 50% probability level.

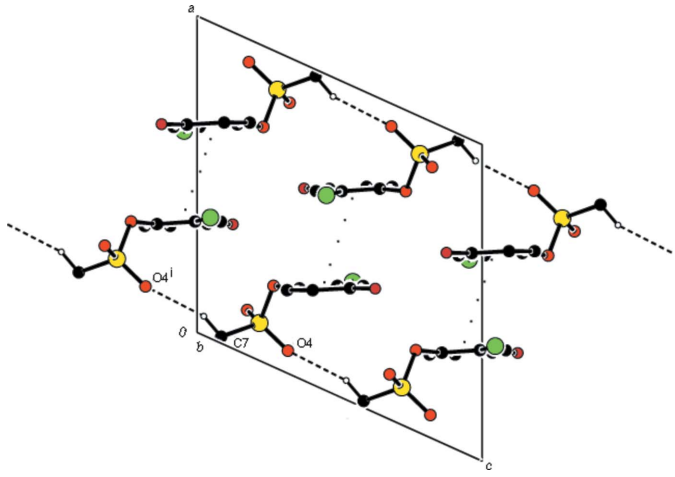

Figure 2
Packing of (I), viewed down the *b* axis, showing π–π stacking interactions (dotted lines) and C—H···O hydrogen bonds (dashed lines). The symmetry code is as in Table 2.

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