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3-Chloro-2-methylbenzene-1-sulfonyl chloride

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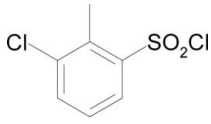
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.047; wR factor = 0.126; data-to-parameter ratio = 19.1.

In the structure of the title compound, $C_7H_6Cl_2O_2S$, the three methyl hydrogen atoms are disordered over two sets of positions with essentially equal occupancy.

Related literature

For related literature, see: Brennan *et al.* (2006).



Experimental

Crystal data

$C_7H_6Cl_2O_2S$
M_r = 225.08
Monoclinic, $C2/c$
a = 11.7233 (16) Å
b = 9.8849 (13) Å
c = 16.216 (2) Å
β = 100.143 (2)°
V = 1849.8 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 293 (2) K
0.50 × 0.44 × 0.33 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.53, T_{max} = 0.76
6310 measured reflections
2101 independent reflections
1551 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.126
S = 1.04
2101 reflections
110 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Data collection: *SCXmini* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku, 2005); software used to prepare material for publication: *CrystalStructure* and *publCIF* (Westrip, 2007).

The authors thank Dr David Lonergan for suggesting a list of possibly crystalline reagents.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2163).

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supplementary materials

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Comment

3-chloro-2-methylbenzenesulfyl derivatives have shown biological activity as hydroxysteroid dehydrogenase inhibitors. These derivatives have potential as medicants to treat diseases mediated by hydroxysteroid dehydrogenase, such as type-2 diabetes (Brennan *et al.*, 2006).

Experimental

The data collection sample was selected directly from many nicely formed specimens found in the bottle from the manufacturer.

Refinement

A Fourier map around the expected positions of the methyl group H atoms clearly indicated two equivalent orientations. Both sets were included (riding model) and their occupancies refined, although the refined value is indistinguishable from 0.50. The C—H distance and C—C—H angles for the methyl H atoms were fixed, but the groups were allowed to rotate around the C—C bond.

Figures

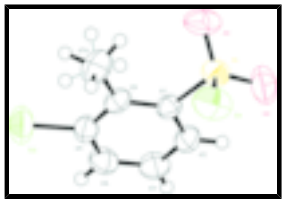

Fig. 1. View of the title molecule, with ellipsoids drawn at the 50% probability level. Bonds to the methyl H atoms are drawn with different line styles to distinguish the two alternate orientations.

3-chloro-2-methylbenzene-1-sulfonyl chloride

Crystal data

$C_7H_6Cl_2O_2S$	F_{000} = 912
M_r = 225.08	D_x = 1.616 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71075 Å
a = 11.7233 (16) Å	Cell parameters from 5438 reflections
b = 9.8849 (13) Å	θ = 3.1–27.5º
c = 16.216 (2) Å	μ = 0.88 mm^{-1}
β = 100.143 (2)º	*T* = 293 (2) K

V = 1849.8 (4) Å^3	Prism, colourless
Z = 8	0.50 × 0.44 × 0.33 mm

Data collection

Rigaku SCXmini diffractometer	1551 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.5º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -15 \rightarrow 15$
T_{min} = 0.53, T_{max} = 0.76	$k = -12 \rightarrow 12$
6310 measured reflections	$l = -16 \rightarrow 20$
2101 independent reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 2.2518P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.126	$\Delta\rho_{max}$ = 0.49 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.47 e Å^{-3}
2101 reflections	Extinction correction: none
110 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)

Cl1	0.34739 (8)	−0.05390 (11)	0.72960 (6)	0.0881 (4)	
Cl2	0.00368 (8)	−0.33397 (9)	0.46807 (7)	0.0842 (3)	
S1	0.22728 (7)	0.07269 (8)	0.66422 (5)	0.0567 (2)	
O1	0.1375 (2)	0.0813 (3)	0.71120 (13)	0.0744 (7)	
O2	0.2877 (3)	0.1917 (3)	0.64869 (16)	0.0909 (8)	
C1	0.1833 (2)	−0.0162 (3)	0.56917 (16)	0.0440 (6)	
C2	0.2169 (3)	0.0433 (3)	0.49984 (19)	0.0553 (7)	
H1	0.2617	0.1214	0.5059	0.077*	
C3	0.1835 (3)	−0.0139 (3)	0.42236 (18)	0.0614 (8)	
H3	0.2052	0.0257	0.3755	0.086*	
C4	0.1182 (3)	−0.1296 (3)	0.41408 (18)	0.0561 (7)	
H2	0.0953	−0.1687	0.3616	0.079*	
C5	0.0868 (2)	−0.1876 (3)	0.48380 (18)	0.0496 (6)	
C6	0.1180 (2)	−0.1350 (3)	0.56484 (16)	0.0450 (6)	
C7	0.0831 (3)	−0.2042 (4)	0.6395 (2)	0.0720 (9)	
H4A	0.1392 (3)	−0.2724 (4)	0.6602 (2)	0.101*	0.51 (4)
H5A	0.0796 (3)	−0.1387 (4)	0.6827 (2)	0.101*	0.51 (4)
H6A	0.0084 (3)	−0.2454 (4)	0.6232 (2)	0.101*	0.51 (4)
H4B	0.0100 (3)	−0.1690 (4)	0.6485 (2)	0.101*	0.49 (4)
H5B	0.0763 (3)	−0.2997 (4)	0.6293 (2)	0.101*	0.49 (4)
H6B	0.1409 (3)	−0.1877 (4)	0.6883 (2)	0.101*	0.49 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0692 (5)	0.1192 (8)	0.0678 (6)	0.0225 (5)	−0.0101 (4)	−0.0142 (5)
Cl2	0.0835 (6)	0.0593 (5)	0.1071 (7)	−0.0258 (4)	0.0097 (5)	−0.0104 (5)
S1	0.0602 (4)	0.0650 (5)	0.0453 (4)	−0.0035 (3)	0.0105 (3)	−0.0092 (3)
O1	0.0691 (14)	0.1077 (19)	0.0487 (12)	0.0131 (13)	0.0169 (10)	−0.0114 (12)
O2	0.121 (2)	0.0754 (15)	0.0774 (16)	−0.0412 (15)	0.0193 (15)	−0.0218 (13)
C1	0.0435 (13)	0.0500 (14)	0.0401 (13)	−0.0022 (11)	0.0115 (11)	0.0021 (11)
C2	0.0644 (17)	0.0526 (16)	0.0533 (16)	−0.0148 (14)	0.0224 (14)	−0.0003 (13)
C3	0.075 (2)	0.071 (2)	0.0429 (15)	−0.0047 (16)	0.0237 (15)	0.0036 (14)
C4	0.0595 (17)	0.0640 (17)	0.0445 (15)	0.0028 (14)	0.0081 (13)	−0.0060 (14)
C5	0.0428 (13)	0.0428 (13)	0.0617 (17)	−0.0012 (11)	0.0051 (12)	−0.0009 (12)
C6	0.0402 (12)	0.0478 (14)	0.0478 (14)	0.0014 (11)	0.0102 (11)	0.0106 (12)
C7	0.079 (2)	0.074 (2)	0.065 (2)	−0.0148 (17)	0.0178 (17)	0.0248 (17)

Geometric parameters (Å, °)

Cl1—S1	2.0363 (12)	C4—C5	1.374 (4)
Cl2—C5	1.738 (3)	C5—C6	1.401 (4)
S1—O1	1.406 (2)	C6—C7	1.508 (4)
S1—O2	1.419 (3)	C7—H4B	0.9600
S1—C1	1.770 (3)	C7—H6A	0.9600
C1—C2	1.386 (4)	C7—H4A	0.9600
C1—C6	1.397 (4)	C7—H5B	0.9600
C2—C3	1.371 (4)	C7—H6B	0.9600
C3—C4	1.370 (4)	C7—H5A	0.9600

O1—S1—O2	119.41 (17)	C1—C6—C5	114.2 (2)
O1—S1—C1	111.75 (13)	C1—C6—C7	124.4 (3)
O2—S1—C1	109.58 (14)	C5—C6—C7	121.5 (3)
O1—S1—Cl1	105.65 (11)	H6A—C7—H4A	109.5
O2—S1—Cl1	106.32 (14)	H6A—C7—H5A	109.5
C1—S1—Cl1	102.52 (10)	H4A—C7—H5A	109.5
C2—C1—C6	123.2 (2)	H4B—C7—H5B	109.5
C2—C1—S1	114.5 (2)	H4B—C7—H6B	109.5
C6—C1—S1	122.28 (19)	H5B—C7—H6B	109.5
C3—C2—C1	119.5 (3)	H4A—C7—C6	109.5
C4—C3—C2	119.9 (3)	H5A—C7—C6	109.5
C3—C4—C5	119.6 (3)	H6A—C7—C6	109.5
C4—C5—C6	123.6 (3)	H4B—C7—C6	109.5
C4—C5—Cl2	116.8 (2)	H5B—C7—C6	109.5
C6—C5—Cl2	119.6 (2)	H6B—C7—C6	109.5

Fig. 1