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4-Allyl-2-methoxyphenyl 3,4-dichlorobenzenesulfonate

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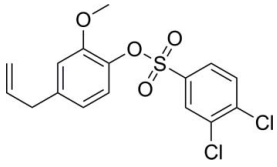
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.048; wR factor = 0.140; data-to-parameter ratio = 14.2.

The title compound, $C_{16}H_{14}Cl_2O_4S$, was obtained by the reaction of eugenol (4-allyl-2-methoxyphenol) and 3,4-dichlorobenzenesulfonyl chloride. The dihedral angle between the benzene rings in the molecule is 40.53 (4)°. No significantly short intermolecular contacts are observed in the crystal structure.

Related literature

For the synthesis of eugenol derivatives, see: Sadeghian *et al.* (2008). For a related structure, see: Ma *et al.* (2010).



Experimental

Crystal data

$C_{16}H_{14}Cl_2O_4S$ M_r = 373.23
Triclinic, $P\overline{1}$
a = 8.8694 (8) Å
b = 9.7501 (9) Å
c = 10.3796 (11) Å
α = 83.369 (2)°
β = 76.196 (1)°
γ = 80.038 (1)°
V = 855.95 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 298 K
0.45 × 0.40 × 0.30 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.801, T_{max} = 0.860
4290 measured reflections
2967 independent reflections
1762 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.140
S = 1.02
2967 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2390).

References

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Sadeghian, H., Seyedi, S. M., Saberi, M. R., Arghiani, Z. & Riazi, M. (2008). *Bioorg. Med. Chem.* **16**, 890–901.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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supporting information

Acta Cryst. (2011). E**67**, o3082 [doi:10.1107/S1600536811044163]

4-Allyl-2-methoxyphenyl 3,4-dichlorobenzenesulfonate

Ya-Tuan Ma, Zhao-Feng Gao, Qi-Chao Liu, Gang Jin and Jin-Ming Gao

S1. Comment

In this paper, we present the structure of the title compound (Fig. 1), which was synthesized by the reaction of eugenol and 3,4-dichlorobenzenesulfonyl chloride (Sadeghian *et al.*, 2008). We previously reported a compound of this type (Ma *et al.*, 2010). In the molecular structure, the bond lengths and angles are normal and the dihedral angle between the aromatic rings is 40.53 (4)°. The crystal packing exhibits no significantly short intermolecular contacts.

S2. Experimental

492 mg of eugenol (3 mmol), triethylamine (4 mmol), 3,4-dichlorobenzenesulfonyl chloride (3 mmol), and 40 ml of dichloromethane were mixed in a 100 ml flask. After 2 h under stirring at 278 K, the crude product was obtained. The crystals were obtained by recrystallization from methanol.

S3. Refinement

The positions of all H atoms were fixed geometrically and C—H bond lengths fixed to 0.93 (aromatic CH), 0.96 (methyl CH_3) or 0.97 Å (methylene CH_2). Isotropic displacement parameters for H atoms were fixed to U_{iso}(H7x) = 1.5U_{eq}(C7) and U_{iso}(H) = 1.2U_{eq}(carrier C) for other H atoms.

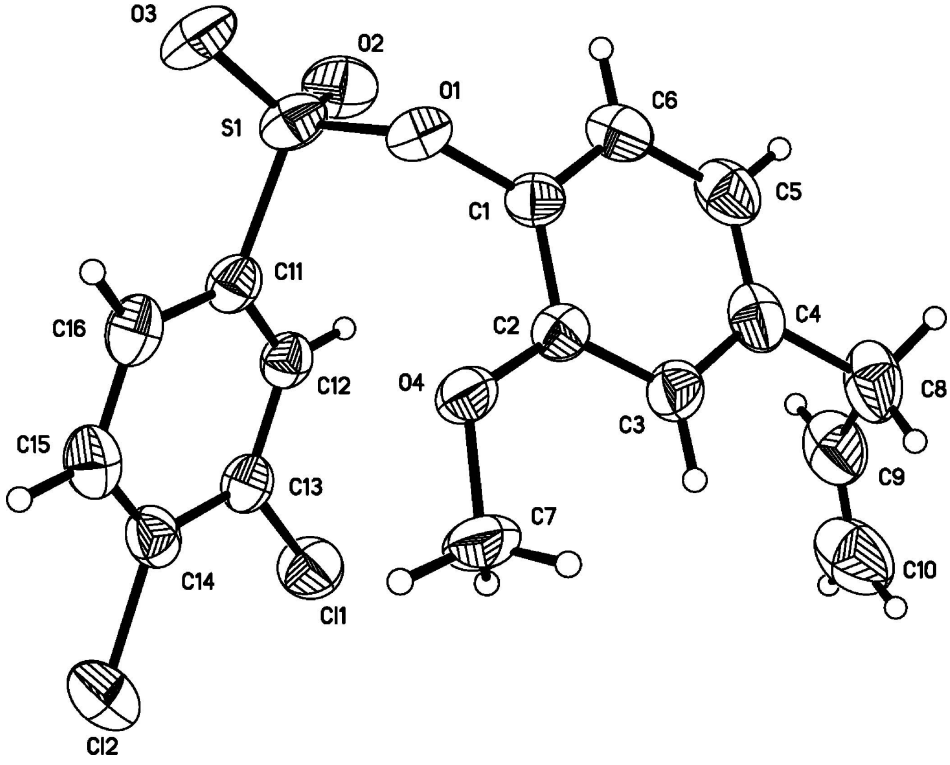

Figure 1

The molecular structure of the title molecule. Displacement ellipsoids are drawn at the 30% probability level.

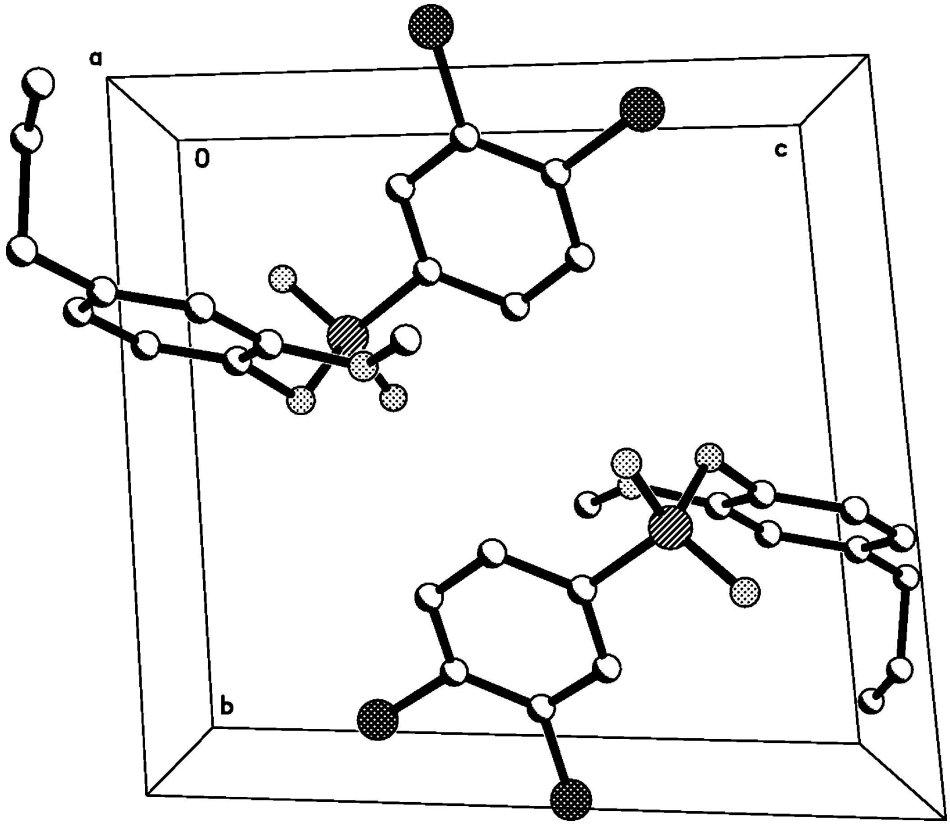

Figure 2

Packing diagram.

4-Allyl-2-methoxyphenyl 3,4-dichlorobenzenesulfonate

Crystal data

$C_{16}H_{14}Cl_2O_4S$
$M_r = 373.23$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.8694$ (8) Å
$b = 9.7501$ (9) Å
$c = 10.3796$ (11) Å
$\alpha = 83.369$ (2)°
$\beta = 76.196$ (1)°
$\gamma = 80.038$ (1)°
$V = 855.95$ (14) Å^3
$Z = 2$
$F(000) = 384$
$D_x = 1.448$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1336 reflections
$\theta = 2.8$–$23.7°$
$\mu = 0.52$ mm^{-1}
$T = 298$ K
Prism, colourless
0.45 × 0.40 × 0.30 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.801$, $T_{max} = 0.860$
4290 measured reflections
2967 independent reflections
1762 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -10 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -9 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.140$
$S = 1.02$
2967 reflections
209 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.4401P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.82040 (13)	0.91886 (11)	1.44301 (11)	0.0879 (4)
Cl2	0.75166 (16)	1.04135 (13)	1.72255 (11)	0.0992 (4)
O1	0.5562 (2)	1.4568 (2)	1.2109 (2)	0.0595 (6)
O2	0.4219 (3)	1.2645 (3)	1.1872 (3)	0.0871 (9)
O3	0.2975 (3)	1.4507 (3)	1.3373 (3)	0.0915 (9)
O4	0.8069 (3)	1.4105 (3)	1.3153 (2)	0.0630 (6)
S1	0.43068 (11)	1.35611 (11)	1.28005 (11)	0.0703 (3)
C1	0.7014 (4)	1.3996 (3)	1.1322 (3)	0.0552 (9)
C2	0.8326 (4)	1.3787 (3)	1.1873 (3)	0.0548 (8)
C3	0.9776 (4)	1.3308 (4)	1.1077 (4)	0.0653 (10)
H3	1.0669	1.3146	1.1428	0.078*
C4	0.9901 (5)	1.3068 (4)	0.9758 (4)	0.0733 (11)
C5	0.8575 (6)	1.3299 (4)	0.9242 (4)	0.0807 (12)
H5	0.8659	1.3141	0.8359	0.097*
C6	0.7135 (5)	1.3759 (4)	1.0020 (4)	0.0716 (11)
H6	0.6244	1.3909	0.9669	0.086*
C7	0.9350 (5)	1.3767 (6)	1.3797 (4)	0.0961 (15)
H7A	0.9763	1.2793	1.3742	0.144*
H7B	0.8993	1.3964	1.4715	0.144*
H7C	1.0157	1.4315	1.3369	0.144*
C8	1.1522 (6)	1.2558 (5)	0.8904 (4)	0.0989 (16)
H8A	1.1523	1.2820	0.7973	0.119*
H8B	1.2304	1.3008	0.9136	0.119*
C9	1.1938 (7)	1.1033 (5)	0.9099 (4)	0.1003 (16)
H9	1.1251	1.0486	0.8940	0.120*
C10	1.3139 (8)	1.0416 (7)	0.9462 (5)	0.133 (2)
H10A	1.3855	1.0926	0.9632	0.159*
H10B	1.3318	0.9445	0.9563	0.159*
C11	0.5144 (4)	1.2605 (4)	1.4070 (3)	0.0578 (9)
C12	0.6161 (4)	1.1383 (4)	1.3789 (3)	0.0564 (9)
H12	0.6347	1.1026	1.2964	0.068*
C13	0.6895 (4)	1.0704 (4)	1.4771 (4)	0.0588 (9)
C14	0.6590 (4)	1.1249 (4)	1.6005 (4)	0.0651 (10)

C15	0.5542 (5)	1.2442 (4)	1.6267 (4)	0.0728 (11)
H15	0.5319	1.2779	1.7105	0.087*
C16	0.4817 (4)	1.3143 (4)	1.5303 (4)	0.0682 (10)
H16	0.4120	1.3965	1.5473	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0900 (8)	0.0784 (7)	0.0890 (8)	0.0078 (6)	−0.0208 (6)	−0.0102 (6)
Cl2	0.1245 (11)	0.1074 (9)	0.0685 (7)	−0.0214 (8)	−0.0319 (7)	0.0095 (6)
O1	0.0484 (14)	0.0575 (14)	0.0743 (16)	0.0003 (11)	−0.0208 (12)	−0.0098 (12)
O2	0.089 (2)	0.091 (2)	0.099 (2)	−0.0254 (16)	−0.0462 (17)	−0.0127 (16)
O3	0.0432 (15)	0.109 (2)	0.120 (2)	0.0058 (15)	−0.0224 (15)	−0.0165 (18)
O4	0.0466 (13)	0.0839 (17)	0.0603 (15)	−0.0047 (12)	−0.0146 (11)	−0.0154 (13)
S1	0.0509 (6)	0.0797 (7)	0.0867 (7)	−0.0086 (5)	−0.0258 (5)	−0.0125 (5)
C1	0.057 (2)	0.049 (2)	0.060 (2)	−0.0025 (16)	−0.0165 (17)	−0.0059 (16)
C2	0.054 (2)	0.049 (2)	0.060 (2)	−0.0053 (16)	−0.0118 (17)	−0.0059 (16)
C3	0.058 (2)	0.061 (2)	0.068 (2)	−0.0009 (18)	−0.0059 (19)	0.0014 (18)
C4	0.086 (3)	0.053 (2)	0.063 (3)	0.005 (2)	0.004 (2)	0.0011 (19)
C5	0.103 (4)	0.074 (3)	0.059 (2)	−0.001 (3)	−0.015 (2)	−0.008 (2)
C6	0.084 (3)	0.068 (3)	0.064 (2)	0.000 (2)	−0.026 (2)	−0.005 (2)
C7	0.057 (2)	0.158 (5)	0.082 (3)	−0.004 (3)	−0.034 (2)	−0.023 (3)
C8	0.101 (3)	0.076 (3)	0.086 (3)	0.011 (3)	0.023 (3)	0.002 (2)
C9	0.109 (4)	0.095 (4)	0.073 (3)	0.018 (3)	0.008 (3)	−0.017 (3)
C10	0.156 (6)	0.141 (5)	0.078 (3)	0.031 (5)	−0.014 (4)	−0.017 (3)
C11	0.048 (2)	0.062 (2)	0.066 (2)	−0.0153 (17)	−0.0104 (17)	−0.0087 (18)
C12	0.051 (2)	0.062 (2)	0.059 (2)	−0.0159 (18)	−0.0095 (17)	−0.0103 (17)
C13	0.054 (2)	0.057 (2)	0.065 (2)	−0.0165 (17)	−0.0068 (18)	−0.0049 (18)
C14	0.070 (2)	0.072 (3)	0.055 (2)	−0.026 (2)	−0.0103 (18)	0.0020 (19)
C15	0.081 (3)	0.076 (3)	0.059 (2)	−0.018 (2)	−0.002 (2)	−0.014 (2)
C16	0.062 (2)	0.066 (2)	0.071 (3)	−0.0100 (19)	0.001 (2)	−0.017 (2)

Geometric parameters (Å, º)

Cl1—C13	1.729 (4)	C7—H7A	0.9600
Cl2—C14	1.724 (4)	C7—H7B	0.9600
O1—C1	1.411 (4)	C7—H7C	0.9600
O1—S1	1.598 (2)	C8—C9	1.471 (6)
O2—S1	1.411 (3)	C8—H8A	0.9700
O3—S1	1.419 (3)	C8—H8B	0.9700
O4—C2	1.356 (4)	C9—C10	1.247 (7)
O4—C7	1.424 (4)	C9—H9	0.9300
S1—C11	1.761 (4)	C10—H10A	0.9300
C1—C6	1.372 (5)	C10—H10B	0.9300
C1—C2	1.390 (4)	C11—C12	1.379 (4)
C2—C3	1.389 (5)	C11—C16	1.387 (5)
C3—C4	1.391 (5)	C12—C13	1.383 (5)
C3—H3	0.9300	C12—H12	0.9300

C4—C5	1.378 (6)	C13—C14	1.391 (5)
C4—C8	1.531 (5)	C14—C15	1.367 (5)
C5—C6	1.371 (6)	C15—C16	1.371 (5)
C5—H5	0.9300	C15—H15	0.9300
C6—H6	0.9300	C16—H16	0.9300

C1—O1—S1	119.2 (2)	H7B—C7—H7C	109.5
C2—O4—C7	117.7 (3)	C9—C8—C4	111.4 (4)
O2—S1—O3	121.23 (17)	C9—C8—H8A	109.4
O2—S1—O1	109.01 (16)	C4—C8—H8A	109.4
O3—S1—O1	102.96 (16)	C9—C8—H8B	109.4
O2—S1—C11	109.38 (17)	C4—C8—H8B	109.4
O3—S1—C11	109.49 (18)	H8A—C8—H8B	108.0
O1—S1—C11	103.13 (14)	C10—C9—C8	125.2 (6)
C6—C1—C2	121.5 (3)	C10—C9—H9	117.4
C6—C1—O1	120.5 (3)	C8—C9—H9	117.4
C2—C1—O1	117.9 (3)	C9—C10—H10A	120.0
O4—C2—C3	125.6 (3)	C9—C10—H10B	120.0
O4—C2—C1	116.1 (3)	H10A—C10—H10B	120.0
C3—C2—C1	118.3 (3)	C12—C11—C16	122.1 (3)
C2—C3—C4	120.3 (4)	C12—C11—S1	119.1 (3)
C2—C3—H3	119.8	C16—C11—S1	118.7 (3)
C4—C3—H3	119.8	C11—C12—C13	118.1 (3)
C5—C4—C3	119.7 (4)	C11—C12—H12	121.0
C5—C4—C8	121.3 (4)	C13—C12—H12	121.0
C3—C4—C8	118.9 (4)	C12—C13—C14	120.1 (3)
C6—C5—C4	120.5 (4)	C12—C13—Cl1	118.9 (3)
C6—C5—H5	119.7	C14—C13—Cl1	121.0 (3)
C4—C5—H5	119.7	C15—C14—C13	120.5 (3)
C5—C6—C1	119.7 (4)	C15—C14—Cl2	119.3 (3)
C5—C6—H6	120.2	C13—C14—Cl2	120.2 (3)
C1—C6—H6	120.2	C14—C15—C16	120.4 (4)
O4—C7—H7A	109.5	C14—C15—H15	119.8
O4—C7—H7B	109.5	C16—C15—H15	119.8
H7A—C7—H7B	109.5	C15—C16—C11	118.8 (4)
O4—C7—H7C	109.5	C15—C16—H16	120.6
H7A—C7—H7C	109.5	C11—C16—H16	120.6

C1—O1—S1—O2	−44.3 (3)	C3—C4—C8—C9	83.8 (5)
C1—O1—S1—O3	−174.3 (2)	C4—C8—C9—C10	−123.3 (6)
C1—O1—S1—C11	71.8 (3)	O2—S1—C11—C12	27.3 (3)
S1—O1—C1—C6	82.4 (4)	O3—S1—C11—C12	162.3 (3)
S1—O1—C1—C2	−102.5 (3)	O1—S1—C11—C12	−88.6 (3)
C7—O4—C2—C3	−8.0 (5)	O2—S1—C11—C16	−155.9 (3)
C7—O4—C2—C1	173.5 (3)	O3—S1—C11—C16	−20.9 (3)
C6—C1—C2—O4	177.7 (3)	O1—S1—C11—C16	88.2 (3)
O1—C1—C2—O4	2.6 (5)	C16—C11—C12—C13	−1.5 (5)
C6—C1—C2—C3	−1.0 (5)	S1—C11—C12—C13	175.2 (2)

O1—C1—C2—C3	−176.0 (3)	C11—C12—C13—C14	0.6 (5)
O4—C2—C3—C4	−177.4 (3)	C11—C12—C13—Cl1	−178.8 (3)
C1—C2—C3—C4	1.0 (5)	C12—C13—C14—C15	1.2 (5)
C2—C3—C4—C5	−0.5 (6)	Cl1—C13—C14—C15	−179.4 (3)
C2—C3—C4—C8	179.2 (3)	C12—C13—C14—Cl2	−179.4 (3)
C3—C4—C5—C6	−0.2 (6)	Cl1—C13—C14—Cl2	−0.1 (4)
C8—C4—C5—C6	−179.9 (4)	C13—C14—C15—C16	−2.2 (6)
C4—C5—C6—C1	0.3 (6)	Cl2—C14—C15—C16	178.5 (3)
C2—C1—C6—C5	0.3 (6)	C14—C15—C16—C11	1.3 (6)
O1—C1—C6—C5	175.2 (3)	C12—C11—C16—C15	0.6 (5)
C5—C4—C8—C9	−96.5 (5)	S1—C11—C16—C15	−176.2 (3)