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Ethyl phenylsulfonylacetate

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Key indicators

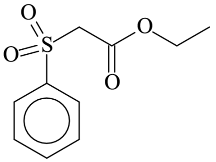
Single-crystal X-ray study
T = 298 K
Mean *σ*(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.098
Data-to-parameter ratio = 12.7

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

The ethyl acetate portion of the molecule of ethyl phenylsulfonylacetate, $C_{10}H_{12}O_4S$, is nearly planar, and it makes a dihedral angle of 44.3 (1)° with the plane of the aromatic ring.

Comment

The synthesis of ethyl phenylsulfonylacetate (I) is an example of microwave-assisted synthesis (Kingston & Haswell, 1997; Loupy, 2002) without the use of a solvent (Loupy *et al.*, 1998). The compound can be alkylated, also under microwave irradiation, without the use of either a catalyst or a solvent (Wang & Jiang, 1992). The structure of the *p*-nitro-substituted derivative has been reported (Anulewicz *et al.*, 1990).



(I)

Bond lengths in ethyl phenylsulfonylacetate (Fig. 1 and Table 1) are similar to those found in the *p*-nitro analog (Anulewicz *et al.*, 1990); in that compound, the almost planar ethyl acetate portion is twisted by 86.5 (1)° with respect to the aromatic ring. In the unsubstituted compound reported here, the corresponding portion is also nearly planar (r.m.s. deviation 0.08 Å), making a dihedral angle of 44.3 (1)° with the plane of the aromatic ring. The crystal structure is stabilized mainly by van der Waals interactions.

Experimental

The compound was prepared by the hydrocarbylation of sodium phenylsulfinate dihydrate, $C_6H_5SO_2Na\cdot 2H_2O$ (2.0 g, 10 mmol), and ethyl bromoacetate (1.2 ml, 11 mmol) in the presence of cetyltrimethylammonium bromide catalyst (1.8 g). The reaction was carried out in a 630 W microwave oven for 1 min. Single crystals were obtained by recrystallization from cyclohexane.

Crystal data

$C_{10}H_{12}O_4S$
$M_r = 228.26$
Monoclinic, $P2_1$
$a = 8.8812$ (3) Å
$b = 5.8066$ (2) Å
$c = 11.5280$ (5) Å
$\beta = 111.583$ (1)°
$V = 552.81$ (4) Å^3
$Z = 2$
$D_x = 1.371$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2044 reflections
$\theta = 2.5$–27.7°
$\mu = 0.28$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.42 × 0.21 × 0.13 mm

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Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: none
3436 measured reflections
2341 independent reflections
2273 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\rm max} = 27.5°$
$h = -10 \rightarrow 11$
$k = -7 \rightarrow 7$
$l = -14 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.098$
$S = 1.08$
2341 reflections
184 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.0130P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.18$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.28$ e Å^{-3}
Absolute structure: Flack (1983); 974 Friedel pairs
Flack parameter = 0.19 (8)

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.431 (2)	O4—C8	1.312 (3)
S1—O2	1.436 (2)	O4—C9	1.465 (2)
S1—C1	1.766 (2)	C7—C8	1.505 (3)
S1—C7	1.792 (2)	C9—C10	1.470 (4)
O3—C8	1.190 (3)		
O1—S1—O2	118.9 (1)	C8—O4—C9	116.8 (2)
O1—S1—C1	108.7 (1)	S1—C7—C8	113.3 (2)
O2—S1—C1	108.5 (1)	O3—C8—O4	125.1 (2)
O1—S1—C7	106.7 (1)	O3—C8—C7	122.3 (2)
O2—S1—C7	108.6 (1)	O4—C8—C7	112.6 (2)
C1—S1—C7	104.4 (1)	O4—C9—C10	108.7 (2)
C9—O4—C8—O3	−1.4 (3)	C8—O4—C9—C10	167.0 (2)
C9—O4—C8—C7	177.5 (2)		

H atoms were located in a difference map and refined with a C—H distance restraint of 0.95 (1) Å. The refinement with the inverted configuration gave an *R* index of 0.039 and a Flack parameter of 0.80 (8).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

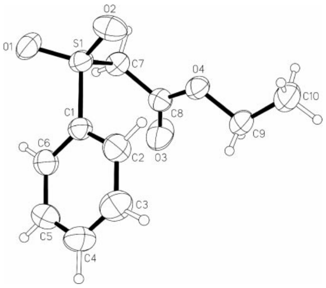

Figure 1
ORTEP (Johnson, 1976) plot of $C_6H_5SO_2CH_2CO_2C_2H_5$, showing 50% probability displacement ellipsoids. H atoms are drawn as spheres of arbitrary radii.

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