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4-[(4-Methoxybenzyl)sulfanyl]benzaldehyde

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.099
Data-to-parameter ratio = 17.8

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

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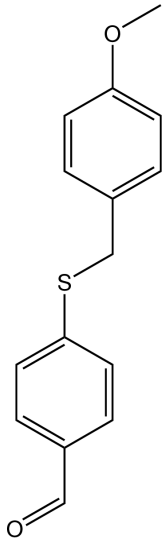
The title compound, $C_{15}H_{14}O_2S$, adopts an extended conformation that enables the formation of $\pi\cdots\pi$ and C—H$\cdots$O contacts in the crystal structure, leading to the formation of columns.

Comment

The title compound, (I) (Fig. 1), adopts an extended conformation as seen in the value of the C4—S4—C41—C42 torsion angle of −172.08 (14)°. The dihedral angle between the least-squares plane through the two aromatic rings is 72.52 (9)°. The observed molecular conformation allows for the formation of columns of molecules, running parallel to *b*, that are stabilized by $\pi\cdots\pi$ interactions occurring between the C1–C6 aromatic rings. Within the columns, the closest contact between the ring centroids of 3.508 (3) Å occurs between centrosymmetrically related molecules (symmetry code: $1-x, 1-y, 1-z$). This pair of molecules forms weaker $\pi\cdots\pi$ interactions to adjacent pairs so that the separation between the ring centroids is 3.764 (3) Å (symmetry code: $1-x, 2-y, 1-z$). Additional stabilization within the columns is provided by C—H$\cdots$O contacts so that H41*A*$\cdots$O11 is 2.57 Å, C41$\cdots$O11 is 3.496 (4) Å and the angle at H41*A* is 155° (symmetry code: $1-x, 2-y, 1-z$). Links between the columns are afforded by C—H$\cdots\pi$ contacts involving H44 and the second aromatic ring C42–C47 at $-\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$ with a H44$\cdots$ring centroid distance of 3.10 Å and the angle at H44 of 136°.



(I)

Experimental

The title compound was obtained by addition of the potassium salt of (4-methoxyphenyl)methane-1-thiol to 4-fluorobenzaldehyde. The product was recrystallized from ethyl acetate/hexane; m.p. 377–378 K. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 3.80, *s*, 3H; 4.20, *s*, 2H; 6.86, *d*, J = 8.7 Hz, 2H; 7.30, *d*, J = 9.0 Hz, 2H; 7.37, *d*, J = 8.4 Hz, 2H; 7.75, *d*, J = 8.7 Hz, 2H; 9.91, *s*, 1H.

Crystal data

$C_{15}H_{14}O_2S$	D_x = 1.345 Mg m^{-3}
M_r = 258.33	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 21 reflections
a = 7.648 (3) Å	θ = 8.4–13.4°
b = 6.872 (6) Å	μ = 0.24 mm^{-1}
c = 24.314 (2) Å	T = 173 K
β = 93.10 (2)°	Plate, colourless
V = 1276.0 (12) Å^3	0.40 × 0.32 × 0.03 mm
Z = 4	

Data collection

Rigaku AFC-7*R* diffractometer	$h = -9 \rightarrow 9$
ω scans	$k = 0 \rightarrow 8$
6267 measured reflections	$l = 0 \rightarrow 31$
2921 independent reflections	3 standard reflections
1671 reflections with $I > 2\sigma(I)$	every 400 reflections
R_{int} = 0.064	intensity decay: −1.2%
θ_{max} = 27.5°	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.099	$(\Delta/\sigma)_{max} < 0.001$
S = 0.97	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
2921 reflections	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
164 parameters	

The C-bound H atoms were placed in geometrically calculated positions and included in the final refinement in the riding-model approximation with an overall displacement parameter.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1996); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1997); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

The Australian Research Council is thanked for support of the crystallographic facility.

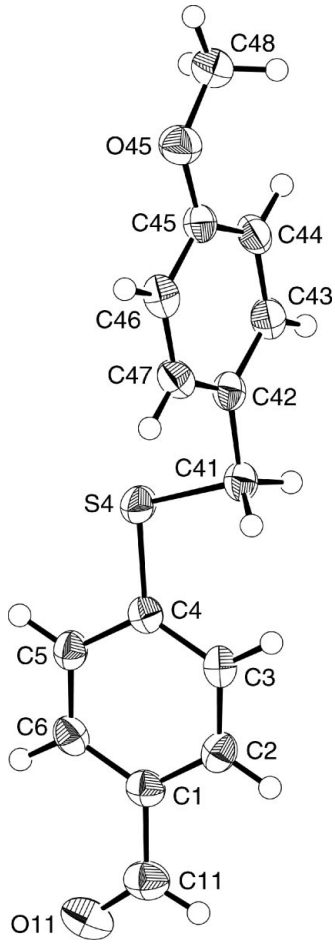


Figure 1
The molecular structure and crystallographic numbering scheme for (I). Displacement ellipsoids are shown at the 50% probability level (Johnson, 1976).

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