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3-[4-(Methylsulfonyl)benzoyl]propionic acid

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.138
Data-to-parameter ratio = 15.6

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

The structure of the title compound, $C_{11}H_{12}O_5S$, (I), comprises a simple molecule that associates *via* carboxylic acid dimers in the solid state. Other associated dimers are formed from C—H···O intermolecular close contacts to the two carbonyl and one sulfonyl O atoms. All three SO_2CH_3 H atoms and one phenyl H atom are also involved in these close-contact associations.

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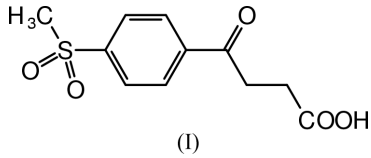

(I)

Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from an ethanol solution.

Crystal data

$C_{11}H_{12}O_5S$
M_r = 256.27
Triclinic, $P\overline{1}$
a = 5.1851 (1) Å
b = 10.5030 (3) Å
c = 10.9550 (4) Å
α = 96.990 (1)°
β = 101.135 (1)°
γ = 101.786 (3)°
V = 564.90 (3) Å^3
Z = 2
D_x = 1.507 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3181 reflections
θ = 2.9–27.5°
μ = 0.29 mm^{-1}
T = 120 (2) K
Prism, colourless
0.40 × 0.20 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.892, T_{max} = 0.983
6362 measured reflections
2484 independent reflections
2089 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°
$h = -6 \rightarrow 6$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

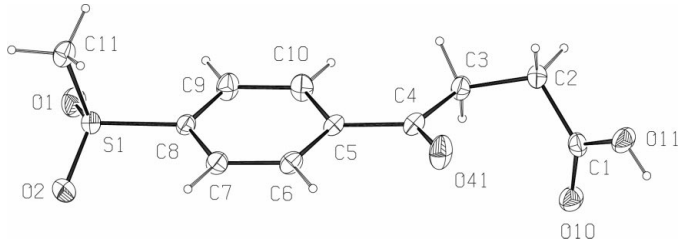

Figure 1
The molecular configuration and atom-numbering scheme for the title compound, showing 50% probability ellipsoids.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.138$
$S = 1.03$
2484 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.66$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O11—H11···O10^{i}	0.79 (3)	1.85 (3)	2.6388 (18)	178 (3)
C6—H6···O41^{ii}	0.95	2.45	3.346 (2)	157
C9—H9···O1	0.95	2.58	2.942 (2)	103
C11—H111···O2^{iii}	0.98	2.50	3.357 (2)	146
C11—H113···O10^{iv}	0.98	2.57	3.483 (2)	155
C11—H112···O2^{v}	0.98	2.49	3.423 (2)	160

Symmetry codes: (i) $1-x, 1-y, -z$; (ii) $1-x, -y, -z$; (iii) $x-1, y, z$; (iv) $x, y-1, z$; (v) $1-x, -1-y, 1-z$.

All H atoms were included in the refinement, at calculated positions, as riding models, with C—H distances set to 0.95 (Ar–H), 0.98 (CH_3) and 0.99 Å (CH_2), except for the carboxylic acid H atom, which was located in a difference synthesis and for which both positional and displacement parameters were refined.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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