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1-[(4-Methylphenyl)sulfonyl]pyrrolidin-2-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.094
Data-to-parameter ratio = 15.1

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

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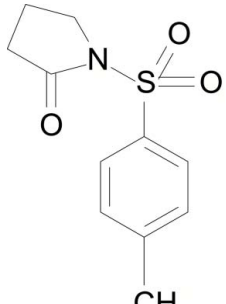
The title molecular structure, $C_{11}H_{13}NO_3S$, contains a five-membered ring which adopts an envelope conformation.

Comment

Sulfonamides are an important class of drugs which are known for their pharmacological activities, *e.g.*, antimicrobial, anti-HIV [amprenavir, a sulfonamide used for the treatment of AIDS and HIV infections (Turner, 2002)], insulin-releasing antidiabetic, carbonic anhydrase inhibitory (Supuran & Scozzafava, 2000, 2001, 2003), high ceiling diuretic, antithyroid and antitumor (Masereel *et al.*, 2002). Keeping in mind the diverse biological activities of sulfonamides, we have synthesized a series of sulfonamides with different functionalities. We report here the structure of the title compound (I), which has been synthesized by dehydrative cyclization of 4-(4-methylphenylsulfonamido)butanoic acid using polyphosphoric ester (Imamoto *et al.*, 1982).



(I)

The crystal structure is composed of discrete molecules of (I) (Fig. 1), packing as shown in Fig. 2. The five-membered pyrrolidine ring adopts an envelope conformation; the flap atom, C10, is 0.392 (3) Å out of the plane formed by the remaining four atoms of the ring. The mean-plane formed by the atoms N1/C8/C9/C11 of the five-membered ring is inclined at 80.19 (9)° with respect to the mean plane of benzene ring C1–C6. The molecular dimensions in (I) are in agreement with the corresponding distances reported for a few structures containing a phenylsulfonylpyrrolidin-2-one fragment in the Cambridge Structural Database (Version 5.27; Allen, 2002), *e.g.* refcodes GUBNOG (Iwamatsu *et al.*, 1999), JIRKOK and JIRLAX (Amato *et al.*, 1990), KONJAY (Bandoli *et al.*, 1992), QACQUH (Benerjee *et al.*, 2002), QELJUM (Clark *et al.*, 1999), SOVDOW and SOVDUC (Amato *et al.*, 1991), and WEPDOK (Taksukawa *et al.*, 1993).

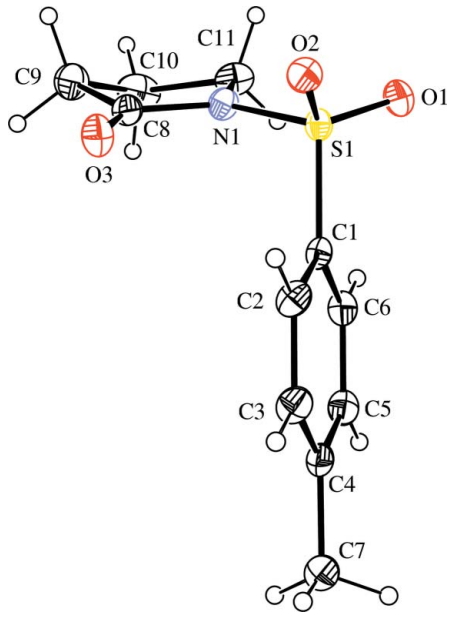


Figure 1
ORTEPII (Johnson, 1976) drawing of (I), with displacement ellipsoids drawn at the 30% probability level; only three of the six H atoms at 0.50 occupancy attached to C7 have been shown.

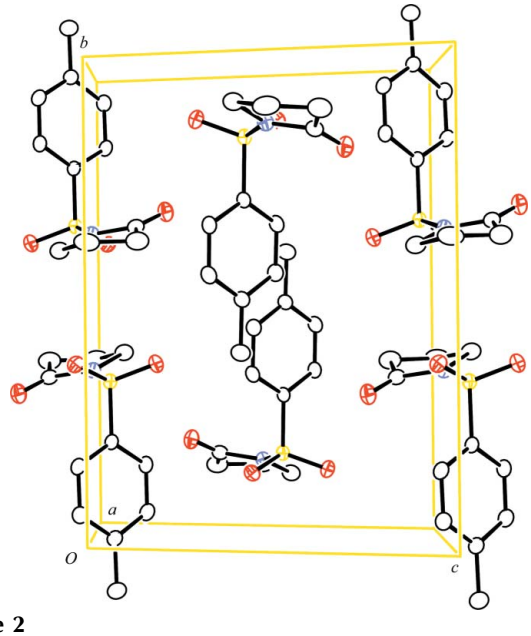


Figure 2
The packing of (I). H atoms have been omitted.

Experimental

The title compound, (I), was synthesized by dehydrative cyclization of 4-(4-methylphenylsulfonamido)butanoic acid with polyphosphoric acid ester (PPE) (Imamoto *et al.*, 1982). A mixture of 4-(4-methylphenylsulfonamido)butanoic acid (1 mmol) and PPE (2 ml) was stirred at room temperature for 17 h. The reaction mixture was treated with saturated aqueous $NaHCO_3$ solution and extracted with chloroform (3 × 10 ml). The combined extract was dried over anhydrous sodium sulfate and evaporated using a rotary evaporator. The product was isolated by preparative thin-layer chromatography on silica gel using ethyl acetate–petroleum ether (1:4) (313–333 K) as eluent. Crystals suitable for an X-ray crystallographic study were grown from a solution of (I) in absolute ethanol by slow evaporation at room temperature.

Crystal data

$C_{11}H_{13}NO_3S$
M_r = 239.28
Monoclinic, $P2_1/n$
a = 8.144 (5) Å
b = 13.717 (10) Å
c = 10.644 (8) Å
β = 108.27 (3)°
V = 1129.1 (14) Å^3
Z = 4
D_x = 1.408 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 173 (2) K
Block, colorless
0.18 × 0.16 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan *SORTAV* (Blessing, 1997)
T_{min} = 0.952, T_{max} = 0.984
3329 measured reflections
2190 independent reflections
1914 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.05
2190 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.606P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.4260 (14)	O3—C8	1.207 (2)
S1—O1	1.4300 (16)	N1—C8	1.392 (3)
S1—N1	1.6604 (17)	N1—C11	1.484 (2)
S1—C1	1.752 (2)		
O2—S1—O1	119.42 (9)	N1—S1—C1	104.58 (7)
O2—S1—N1	108.62 (9)	C8—N1—C11	113.92 (15)
O1—S1—N1	104.46 (9)	C8—N1—S1	123.63 (13)
O2—S1—C1	109.39 (8)	C11—N1—S1	122.45 (13)
O1—S1—C1	109.29 (8)		

H atoms were included in the refinement at geometrically idealized positions, with C—H = 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C); H atoms bonded to C7 are disordered over six sites with equal site-occupancy factors.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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