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2-Morpholino-*N*-(*p*-tolylsulfonyl)ethylamine

Tufan Akbal,[a] Nesuhi Akdemir,[b] Erbil Ağar[b] and Ahmet Erdönmez[a]*

[a]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey, and [b]Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

Correspondence e-mail: takbal@omu.edu.tr

Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.108
Data-to-parameter ratio = 19.1

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

In the crystal structure of the title compound, $C_{13}H_{20}N_2O_3S$, there are some inter- and intramolecular N—H···O, N—H···N and C—H···O hydrogen-bonding interactions.

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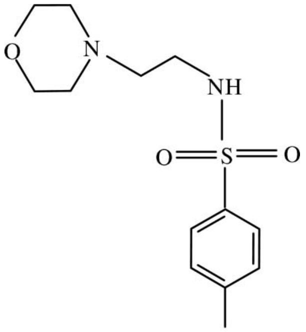
Comment

The title compound, (I), is a derivative of sulfonamide. Sulfonamide derivatives are generally used as antibiotics and photosensitizers for photodynamic therapy (PDT) (Strom *et al.*, 2003; Mak *et al.*, 2003).



(I)

The molecular structure of (I) is shown in Fig. 1and selected geometric parameters are in Table 1. The S1—N1 bond length is in good agreement with data observed in the literature (Öztürk *et al.*, 2000). In the morpholine group, the C11—O3 and C12—O3 bond lengths are consistent with corresponding bonds [1.421 (3) and 1.424 (3) Å] in *erythro*-2-morpholino-1,2-diphenylethanol (Karadayı *et al.*, 2002). The N2—C10 and N2—C13 bond lengths agree with the corresponding values in 1-morpholinomethyl-2-naphthol (Ma *et al.*, 2005) and *erythro*-2-morpholino-1,2-diphenylethanol (Karadayı *et al.*, 2002). The morpholine ring adopts a chair conformation, with puckering parameters of θ = 180.0 (2)°, φ = 259 (12)° and Q_T = 0.567 (2) Å (Cremer & Pople, 1975).

The crystal structure is stabilized by some inter- and intramolecular N—H···O, N—H···N and C—H···O hydrogen-bonding interactions (Fig. 2 and Table 2).

Experimental

2-Morpholinoethylamine (6.45 g, 49.61 mmol) and sodium hydroxide (2.10 g, 52.5 mmol) were dissolved in water (15 ml). A solution of toluene-*p*-sulfonyl chloride (10.15 g, 53.25 mmol) in diethyl ether was added dropwise over 2 h. The mixture was then stirred at room temperature for 10 h. The organic phase was dried over Na_2SO_4 and evaporated. The white product was washed with water and diethyl ether and recrystallization from ethanol gave the title product (yield 12.06 g, 85.05%). Single crystals were obtained from absolute ethanol at room temperature by slow evaporation (m.p. 372–373 K).

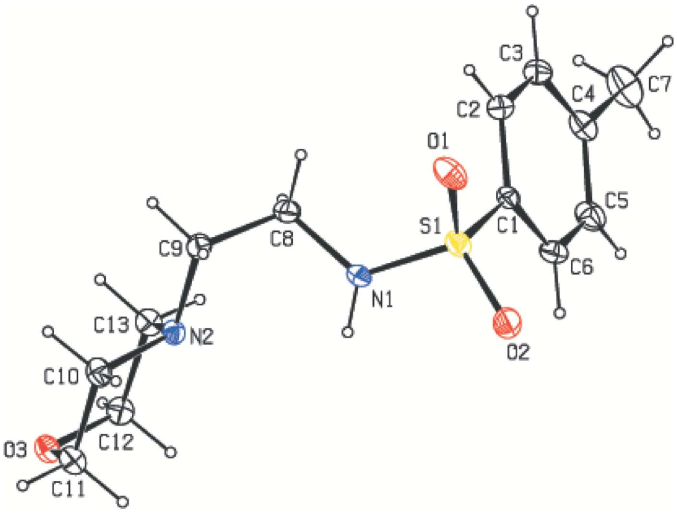


Figure 1
An *ORTEPIII* drawing (Burnett & Johnson, 1996) of (I), showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are shown at the 10% probability level.

Crystal data

$C_{13}H_{20}N_2O_3S$
$M_r = 284.37$
Monoclinic, $P2_1/c$
$a = 13.7639$ (14) Å
$b = 8.0723$ (7) Å
$c = 14.1519$ (15) Å
$\beta = 109.028$ (8)°
$V = 1486.5$ (3) Å^3
$Z = 4$

$D_x = 1.271$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8322 reflections
$\theta = 2.5$–27.4°
$\mu = 0.22$ mm^{-1}
$T = 290$ (2) K
Prism, colourless
0.58 × 0.38 × 0.13 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.975$, $T_{\max} = 0.987$
9234 measured reflections
3303 independent reflections

1888 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.056$
$\theta_{\max} = 27.4°$
$h = -17 \rightarrow 17$
$k = -10 \rightarrow 7$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.108$
$S = 0.90$
3303 reflections
173 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.026 (2)

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.4217 (16)	N2—C13	1.460 (2)
S1—O2	1.4273 (18)	O3—C12	1.419 (3)
S1—N1	1.5966 (18)	O3—C11	1.429 (3)
N2—C10	1.454 (3)		
O1—S1—O2	119.78 (12)	C10—N2—C13	108.86 (17)
N1—S1—C1	108.51 (9)	C12—O3—C11	109.70 (16)
O1—S1—N1—C8	43.81 (19)	C1—S1—N1—C8	−72.04 (17)
O2—S1—N1—C8	172.99 (16)		

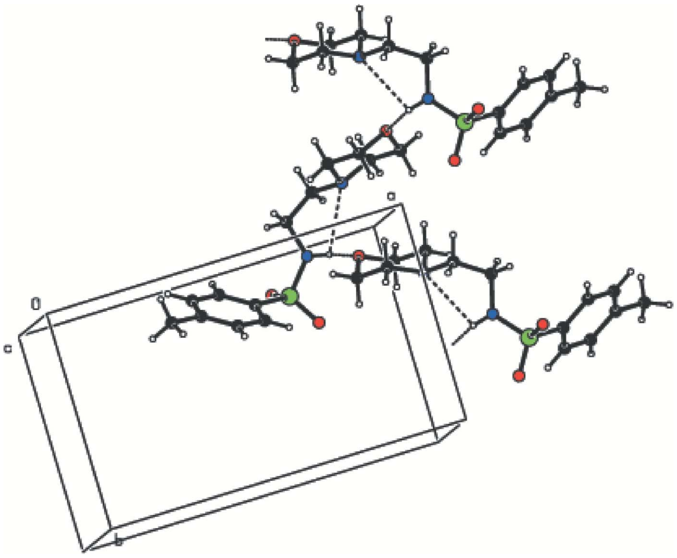


Figure 2
A view of the hydrogen-bonding interactions (dashed lines) in (I).

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H4···O3$^{\rm i}$	0.86	2.20	2.916 (2)	140
C5—H5···O1$^{\rm ii}$	0.93	2.55	3.248 (3)	132
N1—H4···N2	0.86	2.61	2.906 (2)	102
C8—H12B···O1	0.97	2.51	2.949 (3)	107

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å, and with $U_{\rm iso}$(H) constrained to be 1.2 (or 1.5 for methyl H atoms) times $U_{\rm eq}$ of the carrier atom.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

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