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1-(4-Methylphenylsulfonyl)-5-nitro-2-[(*E*)-prop-1-enyl]-1*H*-benzimidazole

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Key indicators

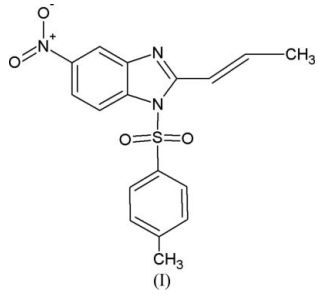
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.088
wR factor = 0.221
Data-to-parameter ratio = 12.8

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

In the title compound, $C_{17}H_{15}N_3O_4S$, the *p*-tolylsulfonyl group is perpendicular to the benzimidazole fragment, and the propenyl group has a *trans* configuration about the olefinic double bond. The molecule is stablized by intramolecular π–π interactions.

Comment

A large number of benzimidizole derivatives have been reported to possess tripanosomicidal actions and are active against diseases caused by protozoa. Some of them have been shown to possess potent and selective activity against *Helicobacter pylori* which is the leading cause of chronic gastritis and peptic ulcer disease and is associated with certain types of gastric cancer (Bjorkholm *et al.*, 2003; Suerbaum & Michetti, 2002). In view of the broad range of medicinal activities of benzimidazole derivatives, the title compound, (I), was synthesized and we report its structure here.



(I)

The benzimidazole fragment (C1–C7/N1/N2) is planar, with a maximum deviation from the mean plane of 0.015 (5) Å for atom C3. The propenyl (C7–C10) and *p*-tolylsulfonyl (C11–C17/S1) fragments are planar, with maximum deviation of 0.038 (1) Å for atom S1 from the least-squares plane of the *p*-tolylsulfonyl fragment. The propenyl fragment makes a dihedral angle of 6.9 (7)° with the benzimidazole ring system. The *p*-tolylsulfonyl fragment is perpendicular to the benzimidazole ring system, with a dihedral angle of 79.9 (2)°. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987).

The molecule is stabilized by intramolecular hydrogen bonds (Table 1). There are also π–π interactions between the imidazole [C1–C7/N1/N2; symmetry code: (i) $-x, 1-y, -z$] and benzene [C1–C6; symmetry code: (ii) $1-x, 1-y, -z$] rings, with a distance between the centroids of 3.532 Å.

Experimental

Equimolar quantities of 4-nitro-1,2-phenylenediamine and crotonic acid were refluxed in 4 *N* HCl to synthesize 5-nitro-2-(prop-1-enyl)benzimidazole as reported previously (Hasan *et al.*, 1990). 5-Nitro-

2-(prop-1-enyl)benzimidazole (1.58 g, 0.007 mol) was dissolved in 10% NaOH (25 ml). A concentrated solution of *p*-tolylsulfonyl chloride (1.38 g, 0.007 mol) in acetone (5 ml) was then added. The mixture was cautiously shaken in a conical flask until complete separation of the product had occurred. The solid product was filtered off, washed with water and recrystallized from ethanol (yield: 70%, 1.95 g; m.p. 417 K).

Crystal data

$C_{17}H_{15}N_3O_4S$
M_r = 357.38
Triclinic, $P\overline{1}$
a = 7.421 (2) Å
b = 9.629 (2) Å
c = 13.144 (4) Å
α = 68.962 (5)°
β = 85.274 (4)°
γ = 71.978 (5)°
V = 833.2 (4) Å^3
Z = 2
D_x = 1.424 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 298 (2) K
Block, colourless
0.33 × 0.23 × 0.21 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.930, T_{max} = 0.954
7818 measured reflections
2923 independent reflections
2056 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.088
$wR(F^2)$ = 0.221
S = 1.17
2923 reflections
228 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0934P)^2 + 0.5296P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3	0.93	2.37	2.920 (6)	118
C8—H8···O4	0.93	2.30	2.940 (7)	126

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl and x = 1.2 for other H atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

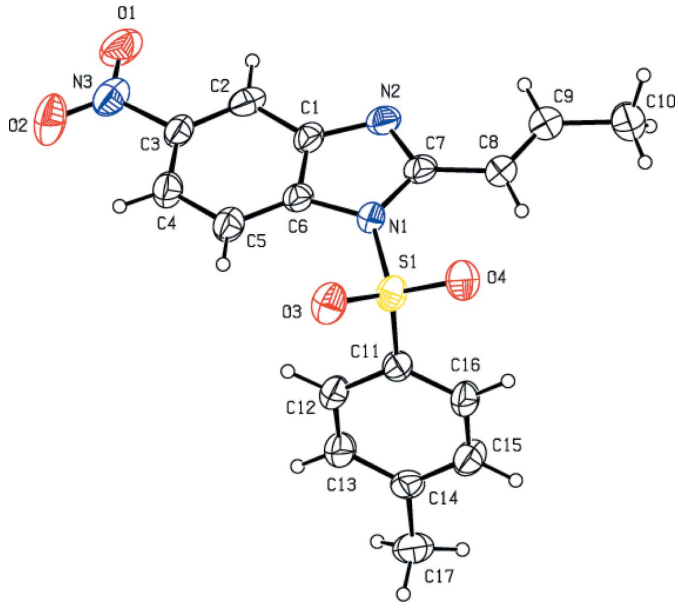


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

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