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2-[2-(Phenylsulfonyl)ethyl]isoindoline-1,3-dione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.080
Data-to-parameter ratio = 14.5

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

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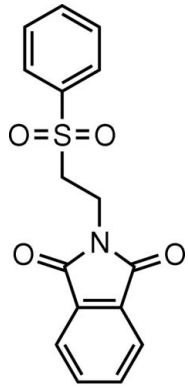
In the title compound, $C_{16}H_{13}NO_4S$, the phthalimide ring system makes a dihedral angle of 56.7 (1) ° with the phenyl ring.

Comment

The title compound, (I), is an intermediate in medicinal synthesis (Ni *et al.*, 2003). The molecular structure of (I) is shown in Fig. 1. In this compound, the phthalimide ring is nearly planar [the maximum deviation from the least-squares plane is 0.021 (1) Å]. Its dimensions are in good agreement with those reported for phthalimide (Matzat, 1972). The phthalimide ring system makes a dihedral angle of 56.7 (1)° with the phenyl ring. Although the molecule contains a phenyl ring and a phthalimide ring system, there are no π–π interactions between molecules.



(I)

Experimental

A mixture of *N*-(2-bromoethyl)phthalimide (1.00 g, 3.95 mmol) and sodium benzenesulfinate dihydrate (2.00 g, 10 mmol) in DMF (50 ml) was stirred at 373 K for 24 h. After cooling to room temperature, the mixture was neutralized by 6 *M* NaOH solution, then extracted with chloroform. The organic layer was separated, then washed with water, and dried over anhydrous magnesium sulfate. The solvent was removed *in vacuo* and the title compound was finally obtained as a white solid. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{16}H_{13}NO_4S$
M_r = 315.33
Orthorhombic, $P2_12_12_1$
a = 5.6147 (6) Å
b = 14.1789 (16) Å
c = 18.483 (2) Å
V = 1471.5 (3) Å^3
Z = 4
D_x = 1.423 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 293 (2) K
Needle, colorless
0.32 × 0.13 × 0.10 mm

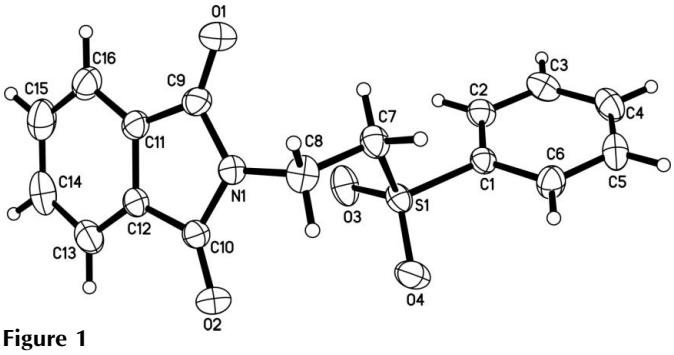


Figure 1
The molecular structure of (I), with the atom-labeling scheme and 30% probability displacement ellipsoids.

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.928, T_{max} = 0.976
8228 measured reflections
2885 independent reflections
2695 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.080
S = 1.06
2885 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.1416P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack (1983), 1187 Friedel pairs
Flack parameter: −0.01 (7)

H atoms were positioned geometrically [C—H = 0.93 (aromatic) or 0.97 Å (CH_2)] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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