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3-Ethylsulfonyl-2-phenylquinoxaline 1,4-dioxide

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.110
Data-to-parameter ratio = 16.8

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

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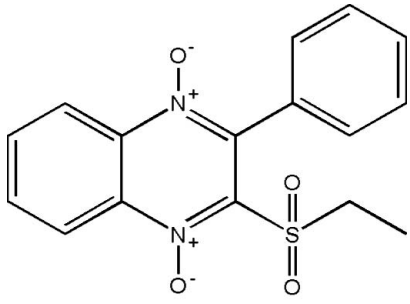
In the title compound, $C_{16}H_{14}N_2O_4S$, the phenyl and quinoxaline 1,4-dioxide planes are approximately perpendicular, with a dihedral angle of 85.8 (2)°.

Comment

Quinoxaline 1,4-dioxides have become an attractive target for organic chemists because of their broad range of biological activities, such as antibacterial (Takabatake *et al.*, 1996), antitubercular (Jaso *et al.*, 2005), cytotoxic (Torre *et al.*, 2005), herbicidal (Ma *et al.*, 2004) and antimalarial (Aldana *et al.*, 2003) activities. In order to study their cytotoxic activity, a series of 2-substituted-phenyl-3-ethylsulfonylquinoxaline 1,4-dioxide has been synthesized. As part of the study, the structure of the title compound, (I), has been determined, and we present the results here.



(I)

In (I), the quinoxaline 1,4-dioxide system is almost planar (Fig. 1 and Table 1). The quinoxaline 1,4-dioxide and phenyl planes are approximately perpendicular, with a dihedral angle of 85.8 (2)°.

Experimental

2-Ethylthioacetophenone (10 mmol) and benzofuroxan (10 mmol) were dissolved in methanol (100 ml) and ammonia gas was bubbled in for 10 min. The reaction mixture was then allowed to stand at room temperature overnight. The crystalline precipitate which formed was filtered off and washed with methanol to give 2-phenyl-3-ethylthioquinoxaline 1,4-dioxide. A solution of *m*-chloroperbenzoic acid (10 mmol) in chloroform (30 ml) was added dropwise to an ice-cold solution of 2-phenyl-3-ethylthioquinoxaline 1,4-dioxide (5 mmol) in chloroform (15 ml), and the reaction mixture was stirred at room temperature overnight. The chloroform solution was washed with aqueous sodium bicarbonate, dried over magnesium sulfate and filtered. After removing the solvent in a vacuum, the residue was purified by crystallization from methanol–chloroform (10:1 *v*/*v*) to

afford the title compound, (I). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol–chloroform solution (25:1 *v*/*v*) of the compound at room temperature.

Crystal data

$C_{16}H_{14}N_2O_4S$
M_r = 330.36
Monoclinic, $P2_1/n$
a = 10.261 (5) Å
b = 8.573 (4) Å
c = 17.898 (7) Å
β = 104.415 (16)°
V = 1524.9 (11) Å^3
Z = 4
D_x = 1.439 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11903 reflections
θ = 3.1–27.5°
μ = 0.23 mm^{-1}
T = 298 (1) K
Prism, brown
0.55 × 0.45 × 0.32 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.859, T_{max} = 0.928
14375 measured reflections
3489 independent reflections
2423 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.026
θ_{max} = 27.5°
$h = -13 \rightarrow 13$
$k = -11 \rightarrow 8$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.01
3489 reflections
208 parameters
H-atom parameters constrained
$w = 1/[0.0009F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O3	1.4245 (15)	S1—C15	1.764 (2)
S1—O4	1.4169 (13)	O1—N1	1.277 (2)
S1—C1	1.8054 (17)	O2—N2	1.2811 (19)
O1—N1—C2—C3	2.8 (2)	N2—C8—C9—C10	−92.2 (2)
O2—N2—C7—C6	−3.7 (2)		

All H atoms were placed in geometrically idealized positions. The methyl H atoms were then constrained to an ideal geometry, with C—H = 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C), but the group was allowed to rotate freely about its C—C bond. Other H atoms were constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 1996); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

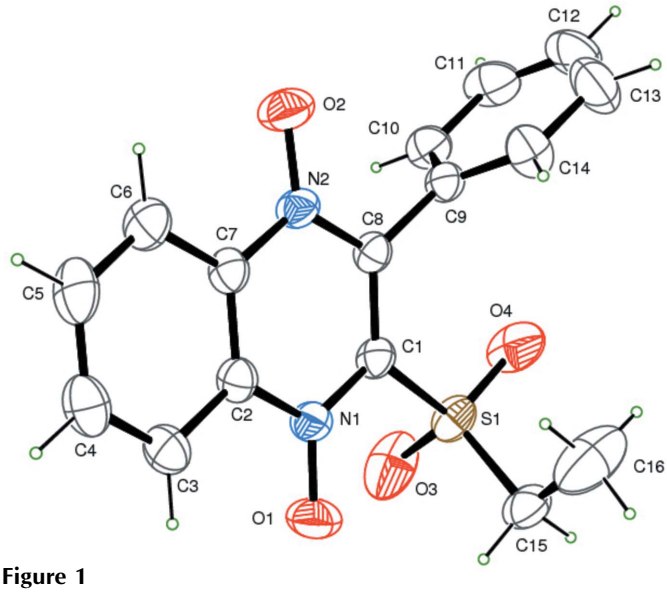


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level.

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