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Ethyl 2-({5-[2-(benzoylamino)phenyl]-1,3,4-oxadiazol-2-yl}sulfanyl)acetate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.125
Data-to-parameter ratio = 16.7

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

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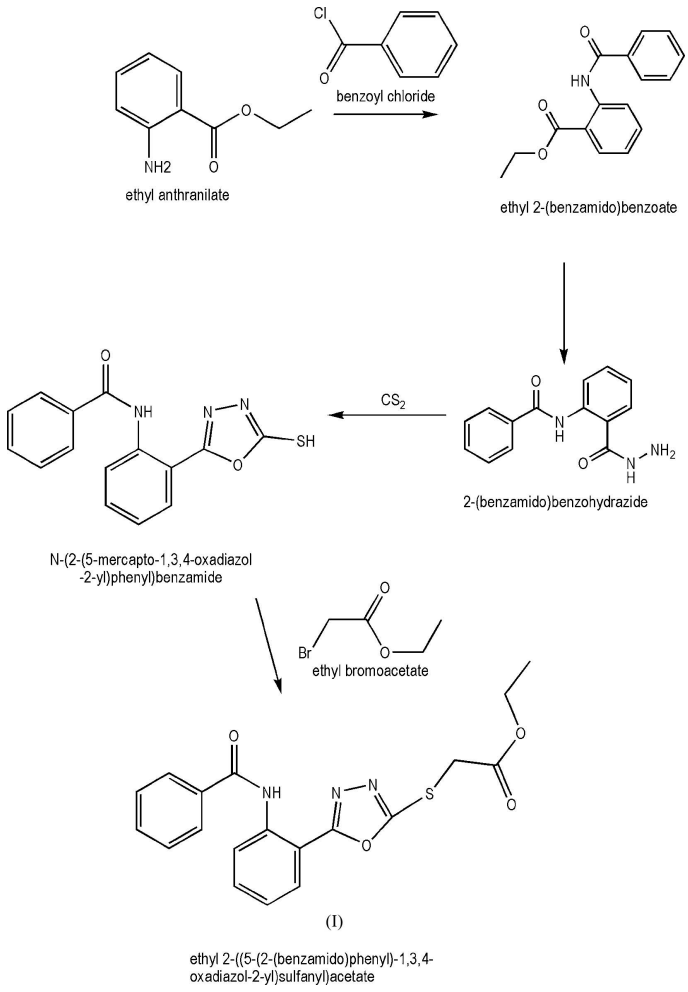
In the title compound, $C_{19}H_{17}O_3N_4S$, a substituted oxadiazole derivative and an important biologically active compound, electron delocalization in the oxadiazole ring is reflected in the C—N bond lengths.

Comment

2,5-Disubstituted-1,3,4-oxadiazoles and their derivatives are of significant interest due to their chemotherapeutic history (Singh *et al.*, 1997). Based on the diverse biological activities of the 2,5-disubstituted-1,3,4-oxadiazoles and their derivatives, we have designed and synthesized some novel oxadiazole derivatives. We report here the structure of the title compound, (I).



In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings *A* (N2/N3/

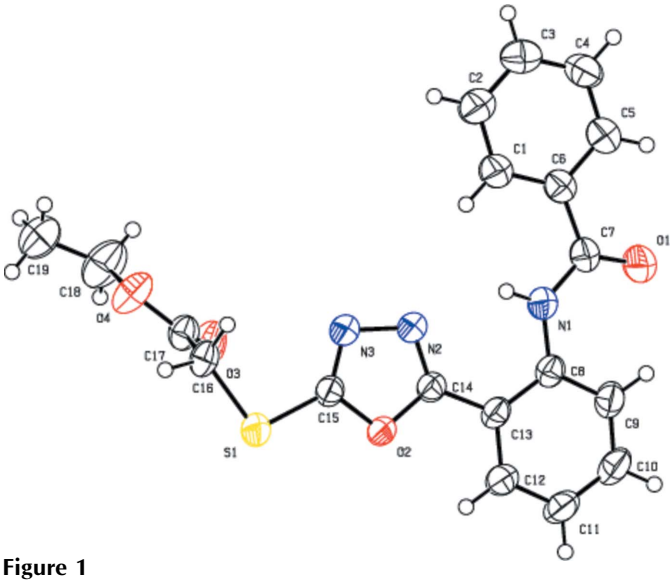


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

O2/C14/C15), *B* (C8–C12) and *C* (C1–C6) are essentially planar. In ring *A*, the N2—C14 [1.291 (3) Å] and N3—C15 [1.280 (3) Å] bonds are longer than a typical C=N double bond and shorter than a typical C—N single bond, indicating electron delocalization in the ring. An intramolecular N1—H1*B*···N2 hydrogen bond is found (Table 1).

Experimental

The title compound, (I), was synthesized in four steps by a reported procedure (Vogel, 1978; Zareef *et al.*, 2006). The amino group of ethyl anthranilate (5.0 g, 30.3 mmol) was protected with benzoyl chloride (7.0 ml, 50 mmol) in basic medium (sodium carbonate, 10 ml). A mixture of *N*-benzoyl ethylanthranilate (2.7 g, 10 mmol) and hydrazine monohydrate (80%) in absolute ethanol (50 ml) was refluxed for 6 h and recrystallized from 60% aqueous ethanol to obtain 2-(*N*-ethylbenzamido)benzohydrazide. 2-(*N*-Ethylbenzamido)benzohydrazide (1.56 g, 5.5 mmol) in 80 ml absolute ethanol was refluxed for 18 h with carbon disulfide (0.50 g, 6.6 mmol) and aqueous potassium hydroxide (0.30 g, 5.5 mmol) to obtain *N*-[2-(5-mercapto-1,3,4-oxadiazol-2-yl)phenyl]benzamide. The title compound, (I), was prepared by reacting *N*-[2-(5-mercapto-1,3,4-oxadiazol-2-yl)phenyl]benzamide (2.97 g, 10 mmol) with ethyl bromoacetate (1.67 g, 10 mmol) in a saturated aqueous sodium bicarbonate solution (30 ml) (yield 81%; m.p. 368–370 K). Crystals suitable for crystallographic study were grown by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{19}H_{17}N_3O_4S$
M_r = 383.42
Orthorhombic, $Pna2_1$
a = 16.810 (3) Å
b = 5.0834 (9) Å
c = 21.274 (4) Å
V = 1818.0 (5) Å^3
Z = 4
D_x = 1.401 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 (2) K
Block, colorless
0.29 × 0.26 × 0.19 mm

Data collection

Bruker SMART CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002\\bb012)
T_{min} = 0.666, T_{max} = 1.000
9147 measured reflections
4085 independent reflections
3693 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 28.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.05
4085 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0857P)^2 + 0.0783P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983). 1772 Friedel pairs.
Flack parameter: 0.08 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*B*···N2	0.86	2.07	2.763 (17)	137

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97, N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C) for amido/aromatic/methylene H atoms or 1.5U_{eq}(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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).

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