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# 1-Ethyl-3-(2-phenylethyl)benzimidazole-2-selone

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**Key indicators**

Single-crystal X-ray study
$T$ = 150 K
Mean $\sigma$(C–C) = 0.005 Å
$R$ factor = 0.042
$wR$ factor = 0.097
Data-to-parameter ratio = 20.9

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



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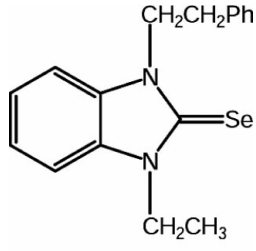
The title compound, $C_{17}H_{18}N_2Se$, was synthesized by heating bis[1-ethyl-3-(2-phenylethyl)benzimidazolidin-2-ylidene] and selenium in toluene. The dihedral angle between the benzimidazole ring system and the phenyl ring is 17.2 (2)°.

## Comment

In recent years, considerable attention has been given to the synthesis of new benzimidazole compounds. In particular, the synthesis of the anti-ulcer drug omeprazole, which contains the benzimidazole moiety, has promoted studies in this area (Carlsson *et al.*, 2002). On the other hand, selenium-containing compounds may play some important role in biological systems, depending on the species (Küçükbay & Demir, 2001). Tetraaminoethylenes are strong reducing agents and react with selenium to give cyclic selenoureas in high yield. We have also synthesized and elucidated the crystal structure of some cyclic selenoureas and related compounds (Aydın *et al.*, 1999; Íngeç *et al.*, 1999; Çetinkaya *et al.*, 1996) and screened them for *in vitro* antimicrobial activities against the standard strains: *Enterococcus faecalis* (ATCC 29212), *Staphylococcus aureus* (ATCC 29213), *Escherichia col*i (ATCC 25922), *Pseudomonas aeruginosa* (ATCC 27853) and the yeasts *Candida albicans* and *Candida tropicalis* (Çetinkaya *et al.*, 1996; Küçükbay & Durmaz, 1997). The objectives of the present study were to elucidate the crystal structure of the recently synthesized title compound, (I) (Küçükbay *et al.*, 2003), and compare the results with those of related cyclic urea derivatives reported previously (Aydın *et al.*, 1999; Íngeç *et al.*, 1999).




(I)

The molecular structure of (I) is shown in Fig. 1. Selected bond lengths and angles are listed in Table 1. The Se1—C1 bond length of 1.829 (3) Å is similar to that [1.825 (7) Å] found in 1,3-dimethylbenzimidazole-2-selone (Aydın *et al.*, 1999). The mean value of the N—C bond lengths in (I) is 1.374 (4) Å, and this and the values of the other geometric parameters are in agreement with the literature data (Aydın *et al.*, 1998; Allen *et al.*, 1987). The benzimidazole ring system (C2–C7/N1/C1/N2) of (I) is planar (r.m.s deviation of fitted atoms is 0.01 Å). The dihedral angle between the phenyl ring

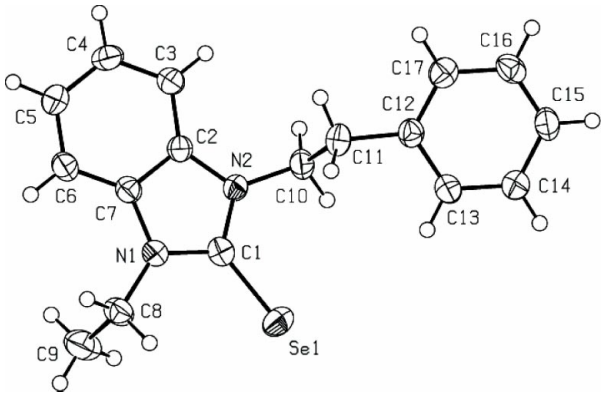



**Figure 1**
An *ORTEP*-3 (Farrugia, 1997) drawing of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

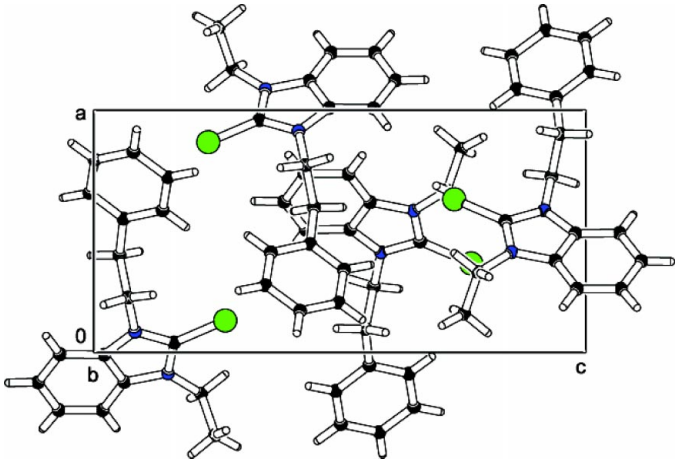



**Figure 2**
A view, down the *b* axis, of the packing of (I).

(C12–C17) and the benzimidazole ring is 17.2 (2)°. A view of the molecular packing in (I) is presented in Fig. 2.

## Experimental

A mixture of bis[1-ethyl-3-(2-phenylethyl)benzimidazolidin-2-ylidene] (1.0 g, 2.00 mmol) and selenium (0.33 g, 4.24 mmol) in toluene (10 ml) was heated under reflux for 2 h. Then the mixture was filtered to remove unreacted selenium and all volatiles were removed *in vacuo* (0.02 mmHg). The crude product was crystallized from alcohol upon cooling to 243 K (yield: 1.16 g, 87%; m.p. 376–377 K). $^1$H NMR (TFA): $\delta$ 0.4 (*t*, $CH_3$, 3H), 2.0 (*t*, $CH_2CH_2Ph$, 2H), 3.4 (*q*, $CH_2CH_3$, 2H), 3.7 (*t*, $CH_2CH_2Ph$, 2H), 5.8–6.2 (*m*, Ar-H, 4H), 6.7 (*s*, Ar-H, 5H). $^{13}$C NMR ($CDCl_3$): $\delta$ 13.72, 34.70, 41.96, 43.05, 109.90, 110.00, 123.62, 123.63, 127.20, 129.10, 129.42, 132.80, 133.46, 138.39, 165.31. $\nu_{(C=Se)}$: 1487 cm$^{-1}$. Analysis calculated for $C_{17}H_{18}N_2Se$: C 60.95, H 5.08, N 8.85%; found: C 60.76, H 5.08, N 9.03%.

*Crystal data*

$C_{17}H_{18}N_2Se$
$M_r$ = 329.29
Orthorhombic, $P2_12_12_1$
$a$ = 7.6427 (5) Å
$b$ = 12.7380 (12) Å
$c$ = 15.5045 (9) Å
$V$ = 1509.41 (19) Å$^3$
$Z$ = 4
$D_x$ = 1.449 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2270 reflections
$\theta$ = 2.1–29.0°
$\mu$ = 2.48 mm$^{-1}$
$T$ = 150 K
Prism, colorless
0.31 × 0.26 × 0.22 mm

*Data collection*

Stoe IPDS-II diffractometer
$\omega$ scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{min}$ = 0.514, $T_{max}$ = 0.612
13746 measured reflections
3831 independent reflections
2914 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.087
$\theta_{max}$ = 28.9°
$h = -10 \rightarrow 10$
$k = -17 \rightarrow 17$
$l = -19 \rightarrow 21$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.097
$S$ = 1.03
3831 reflections
183 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.3896P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0095 (13)
Absolute structure: Flack (1983); 1584 Friedel pairs
Flack parameter = 0.288 (13)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Se1—C1 | 1.829 (3) | N2—C1 | 1.360 (4) |
| N1—C1 | 1.371 (4) | N2—C2 | 1.377 (4) |
| N1—C7 | 1.399 (4) | N2—C10 | 1.456 (4) |
| N1—C8 | 1.459 (4) | | |
| C1—N1—C7 | 109.3 (3) | N1—C1—N2 | 106.6 (3) |
| C1—N1—C8 | 125.4 (3) | N2—C2—C3 | 131.3 (3) |
| C7—N1—C8 | 125.4 (3) | N2—C2—C7 | 107.1 (3) |
| C1—N2—C2 | 110.4 (3) | N1—C7—C2 | 106.6 (3) |
| C1—N2—C10 | 123.7 (3) | N1—C7—C6 | 131.1 (3) |
| C2—N2—C10 | 125.7 (3) | N1—C8—C9 | 112.9 (3) |
| Se1—C1—N1 | 126.3 (2) | N2—C10—C11 | 112.1 (3) |
| Se1—C1—N2 | 127.0 (2) | | |
| C7—N1—C1—Se1 | 179.9 (3) | C2—N2—C10—C11 | −83.4 (4) |
| C8—N1—C1—Se1 | −1.3 (5) | N2—C10—C11—C12 | −164.8 (3) |
| C1—N1—C8—C9 | 96.3 (4) | C10—C11—C12—C13 | 63.8 (4) |
| C7—N1—C8—C9 | −85.1 (4) | C10—C11—C12—C17 | −115.3 (4) |
| C1—N2—C10—C11 | 91.3 (4) | | |

H atoms were placed in geometrically idealized positions (C—H = 0.93–0.97 Å) and allowed to ride on their parent C atoms, with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H atoms and 1.2$U_{eq}$(C) for other H atoms. The Flack parameter indicates partial inversion twinning.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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