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N-(5-Phenylseleno)pentylphthalimide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.035
wR factor = 0.098
Data-to-parameter ratio = 14.6

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

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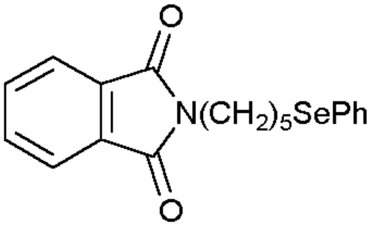
Molecules of the title compound, $C_{19}H_{19}NO_2Se$, are linked into centrosymmetric dimers *via* hydrogen bonds of the C—H···O type. There is also a weak π–π stacking interaction between parallel phthalimide groups belonging to neighbouring dimers in the crystal. The selenopentyl group has a planar zigzag conformation and is approximately coplanar with the phenyl ring. The phthalimide plane forms a dihedral angle of 80.46 (7)° with the least-squares plane of the phenylselenopentyl moiety.

Comment

Oxidation–fragmentation of organoselenides is a useful reaction in organic synthesis (Reich *et al.*, 1978). In order to further investigate the effect of substituents on the course of the reaction, compound (I) was prepared. Its crystal and molecular structure is reported here (Fig. 1).



(I)

The selenopentyl chain in molecule (I) has a typical planar (within 0.06 Å) zigzag conformation. It is, in fact, coplanar with the Ph ring bonded to the Se atom, so that the deviations of atoms from the least-squares plane passing through atoms Se1 and C9–C19 do not exceed 0.06 Å. The dihedral angle formed by this plane and the plane of the phthalimide group is 80.46 (7)°

The crystal packing of (I) features centrosymmetric dimers held together by hydrogen bonds of the C—H···O type [C6—H6*A*···O2^{i}: H6*A*···O2^{i} 2.56 Å, C6···O2^{i} 3.410 (4) Å and C6—H6*A*···O2^{i} 152°; symmetry code: (i) $-x$, $1-y$, $1-z$]. No such interactions, however, were found in the structure of the similar tellurium derivative *N*-[2-(4-methoxyphenyl)telluro]ethylphthalimide (Singh *et al.*, 2000). A weak π–π stacking interaction between two parallel phthalimide groups belonging to neighbouring hydrogen-bonded dimers is also observed in the crystal of (I). The phthalimide moieties are stacked in a head-to-tail fashion with a small offset relative to each other. The distance between the parallel phthalimide planes is 3.728 (4) Å.

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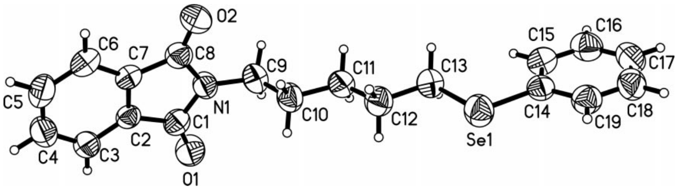

Figure 1
Atom-labelling scheme in structure (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

Experimental

5-Bromopentylphthalimide (1.0 g, 3.2 mmol) and potassium phthalimide (6.1 g, 3.6 mmol) were mixed in DMF (20 ml). The mixture was heated to 368–373 K under nitrogen and stirred for 8 h. It was then cooled to room temperature, diluted with water (20 ml) and extracted with chloroform. The chloroform layer was washed in turn with water, a solution of 10% NaOH and again water, dried over anhydrous magnesium sulfate, filtered and evaporated. The light-yellow residue was recrystallized from a 1:1 mixture of dichloromethane and petroleum ether (303–333 K). Colourless crystals of (I) were obtained (0.96 g, 2.6 mmol, 82%).

Crystal data

$C_{19}H_{19}NO_2Se$
$M_r = 372.31$
Monoclinic, $P2_1/n$
$a = 8.481$ (2) Å
$b = 18.196$ (5) Å
$c = 11.265$ (3) Å
$\beta = 99.361$ (5)°
$V = 1715.3$ (8) Å^3
$Z = 4$

$D_x = 1.442$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 60 reflections
$\theta = 2.4$–30.2°
$\mu = 2.20$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.558$, $T_{\max} = 0.668$
7064 measured reflections

3033 independent reflections
1819 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.030$
$\theta_{\max} = 25.0°$
$h = -9 \rightarrow 10$
$k = -21 \rightarrow 21$
$l = -7 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.098$
$S = 0.94$
3033 reflections
208 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.027$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Se1—C13	1.938 (3)	N1—C8	1.401 (4)
Se1—C14	1.908 (3)	N1—C9	1.459 (4)
O1—C1	1.202 (4)	C1—C2	1.481 (4)
O2—C8	1.207 (4)	C2—C7	1.367 (4)
N1—C1	1.396 (4)	C7—C8	1.476 (4)
C14—Se1—C13	102.42 (15)	C7—C2—C1	109.0 (3)
C1—N1—C8	111.3 (3)	C3—C2—C1	129.2 (3)
C1—N1—C9	124.8 (3)	C2—C7—C8	108.1 (3)
C8—N1—C9	123.8 (3)	O2—C8—N1	123.7 (3)
O1—C1—N1	124.8 (3)	O2—C8—C7	130.2 (3)
O1—C1—C2	129.7 (3)	C15—C14—Se1	124.3 (3)
N1—C1—C2	105.5 (3)	C19—C14—Se1	116.8 (3)
C8—N1—C1—O1	179.4 (3)	C9—N1—C8—O2	3.3 (5)
C9—N1—C1—O1	−3.7 (5)	C9—N1—C8—C7	−176.1 (3)
C8—N1—C1—C2	−0.3 (4)	C8—N1—C9—C10	77.5 (4)
C9—N1—C1—C2	176.7 (3)	C11—C12—C13—Se1	−177.7 (2)
O1—C1—C2—C7	179.9 (4)	C14—Se1—C13—C12	175.7 (2)
N1—C1—C2—C3	−179.5 (3)	C13—Se1—C14—C19	177.2 (3)
C7—C2—C3—C4	0.3 (5)	Se1—C14—C15—C16	179.2 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6A···O2$^{\rm i}$	0.93	2.56	3.410 (4)	152

Symmetry code: (i) $-x, 1-y, 1-z$.

All H atoms were placed in geometrically calculated positions and included in the final refinement in the riding-model approximation with their displacement parameters equal to $1.2U_{\rm eq}$ of the carrier atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SHELXTL* (Sheldrick, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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