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N-(2-Phenethyl)phthalimide

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Key indicators

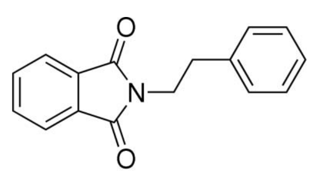
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.095
Data-to-parameter ratio = 12.0

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

The molecule of the title compound, $C_{16}H_{13}NO_2$, contains two planar units, *viz*. a phthalimide system and a phenyl ring in almost parallel orientation, linked by an ethylene bridge. In the crystal structure, the molecules form centrosymmetric pairs which are held together by π–π interactions between the phthalimide systems. The latter are stacked in a head-to-tail fashion with an interplanar distance of 3.263 (6) Å.

Comment

N-(2-Phenethyl)phthalimide (2-phenethylisoindoline-1,3-dione) (I), known from early communications on the Gabriel synthesis (Ing & Manske, 1926), has received new attention as a possible agent in chemotherapy owing to its thalidomide-like effect on the production of the human tumour necrosis factor TNF-α (Sasaki *et al.*, 1995). Consequently, new synthetic approaches to this class of phthalimides have been published, such as the photoinduced electron transfer (PET) of phthalimide anions and arylalkenes (Suau *et al.*, 2003).



(I)

We have recently examined the photochemical properties of (I) in a laser flash photolysis study of the mechanism of PET reactions involving photo-Kolbe and pseudo-photo-Kolbe decarboxylation processes (Warzecha *et al.*, 2006).

The molecular structure of (I) is shown in Fig. 1. The molecule contains two planar subunits, *viz*. the phthalimide chromophore and a phenyl ring, which are linked by an ethylene bridge. The latter shows a staggered conformation with an N1—C9—C10—C11 torsion angle equal to −176.69 (13)°. The C1—N1—C9—C10 and C9—C10—C11—

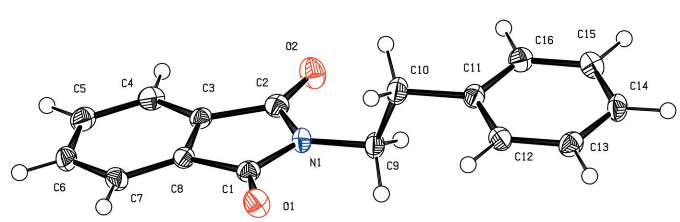


Figure 1
The molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level; H-atoms are shown as circles of arbitrary size.

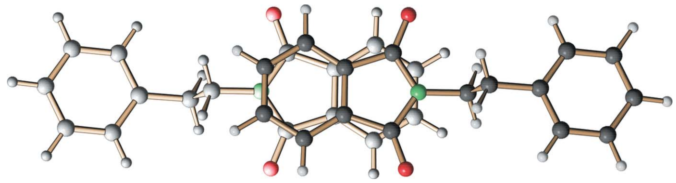


Figure 2
Head-to-tail stacking of phthalimide fragments of two neighbouring molecules in the structure of (I).

C12 torsion angles are close to 90° [−85.46 (17) and −89.71 (17)°, respectively], the ethylene bridge plane being almost orthogonal to both the phthalimide and the phenyl planes.

The crystal packing features pairs of molecules related by an inversion centre with parallel phthalimide planes at a distance of 3.263 (6) Å from each other. In these pairs, the distance between the centre of the six-membered ring of one molecule and the centre of the five-membered ring of the other molecule is as short as 3.447 (1) Å, which implies significant π–π stacking interaction (Fig. 2).

Experimental

A mixture of phthalic anhydride (5.92 g, 40 mmol) and 2-phenethylamine (4.84 g, 40 mmol) in an open beaker was subjected to four cycles of 1 min heating and subsequent cooling in a domestic microwave oven (800 W). Recrystallization of the resulting crude material from ethanol furnished colourless platelets of the title compound (9.04 g, 36 mmol, 90%). An almost equidimensional block suitable for X-ray diffraction, was cut from a thick platelet (m.p. 401 K).

Crystal data

$C_{16}H_{13}NO_2$
M_r = 251.27
Orthorhombic, *Pbca*
a = 28.3243 (9) Å
b = 11.4545 (3) Å
c = 7.6680 (2) Å
V = 2487.81 (12) Å^3
Z = 8
D_x = 1.342 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10877 reflections
θ = 2.3–27.0°
μ = 0.09 mm^{-1}
T = 100 (2) K
Block cut from a thick platelet, colourless
0.42 × 0.40 × 0.40 mm

Data collection

Nonius KappaCCD diffractometer
φ/ω scans
Absorption correction: none
10877 measured reflections
2700 independent reflections
1790 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.067
$\theta_{\rm max}$ = 27.0°
$h = -36 \rightarrow 27$
$k = -14 \rightarrow 12$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.095
S = 0.99
2700 reflections
225 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.019
$\Delta\rho_{\rm max}$ = 0.21 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0058 (8)

All H atoms were refined freely [C—H = 0.952 (16)–1.030 (16) Å].

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SCHAKAL99* (Keller, 1999); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *enCIFer* (Allen *et al.*, 2004).

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