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N-Benzylphthalimide

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Key indicators

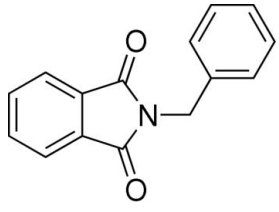
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.108
Data-to-parameter ratio = 11.7

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

In the roof-shaped molecule of the title compound, $C_{15}H_{11}NO_2$, a planar cyclic imide and a phenyl ring are tethered by a methylene group. In the crystal structure, parallel layers of phthalimides stack along the *a* axis with interplanar distances of 3.394 (2) and 3.495 (2)Å.

Comment

N-Benzylphthalimide (2-benzylisoindoline-1,3-dione), (I), the lower homologue of the previously described *N*-(2-phenethyl)phthalimide (Warzecha, Lex *et al.*, 2006) was prepared for a mechanistic study on photoinduced electron transfer (PET) reactions with phthalimides as electron acceptors and arylalkyl carboxylates as electron donors (Warzecha, Görner & Griesbeck, 2006).



(I)

In the course of these synthetically valuable phototransformations, excitation (λ_{exc} = 300 nm) of the phthalimide furnishes its triplet state. Subsequent single electron transfer between the donor and the electronically excited acceptor reduces the phthalimide to its radical anion, thereby oxidizing the arylalkyl carboxylate to the corresponding acyloxy radical. Spontaneous decarboxylation of the latter, followed by recombination of the radical intermediates, gives rise to products identical to those obtained thermally in Grignard-type reactions.

The structure of the title compound, (I), is shown in Fig. 1. The molecule consists of two planar subunits, *viz*. the phthalimide chromophore and a phenyl ring, linked *via* the sp^3-centre C9. The N1—C9—C10 bond angle is 111.18 (13)°.

The C1—N1—C9—C10 and C2—N1—C9—C10 torsion angles from the carbonyl atoms to the benzyl substituent are close to 90° [−86.21 (18) and 90.09 (18)°, respectively]. The pair of torsion angles from the imide N atom to the phenyl ring are virtually the same: N1—C9—C10—C11 = 90.73 (18)° and N1—C9—C10—C15 = −86.82 (16)°. As a result, the title compound exhibits a roof-shaped conformation.

The crystal packing features stacking of the molecules along the crystallographic *a* axis. The centroid–centroid distances from the centre of the five-membered ring of one phthalimide

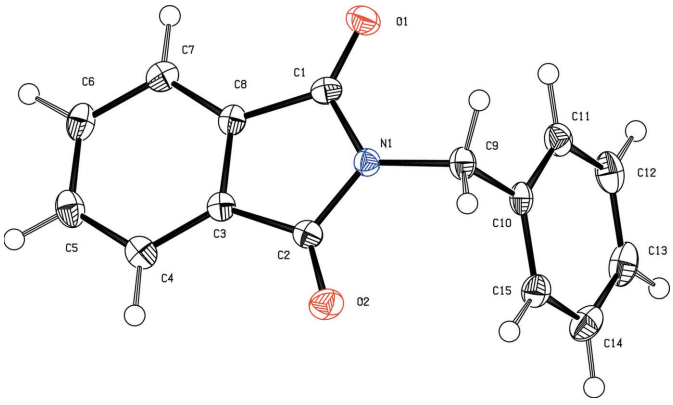


Figure 1
The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as circles of arbitrary size.

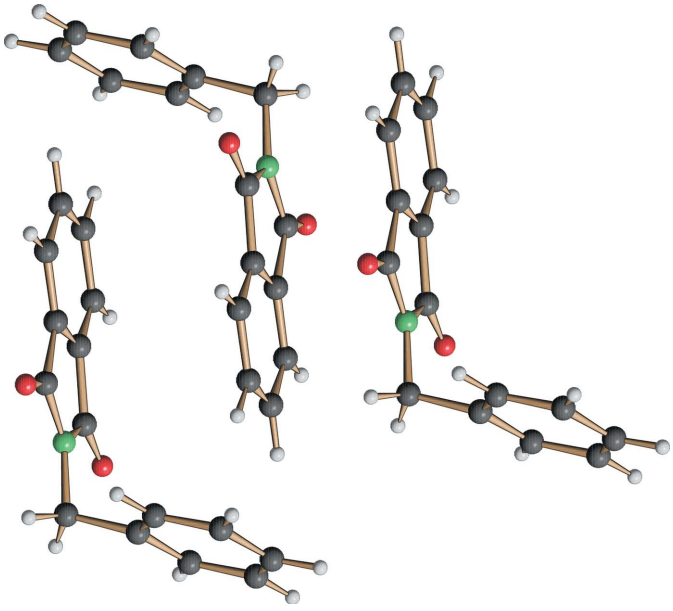


Figure 2
Stacking of the phthalimides along the crystallographic *a* axis.

to the centres of the six-membered rings of the next neighbours above and below are 3.751 (1) and 3.862 (1)Å, respectively. The phthalimides are oriented in parallel layers with interplanar distances of 3.394 (2) and 3.495 (2) Å.

Experimental

The title compound was prepared by heating equimolar amounts of phthalic anhydride and benzylamine in an open beaker for five successive one-minute periods in a domestic microwave oven (800 W). The liquefied material was carefully treated with acetone and the insoluble residue filtered off. Treament of the filtrate with water caused precipitation of the crude imide. Subsequent recrystallization from ethanol yielded colourless prisms (m.p. 384–385 K) suitable for X-ray diffraction.

Crystal data

$C_{15}H_{11}NO_2$	V = 566.88 (4) Å^3
M_r = 237.25	Z = 2
Triclinic, $P\overline{1}$	D_x = 1.390 Mg m^{-3}
a = 7.1159 (3) Å	Mo $K\alpha$ radiation
b = 8.4691 (3) Å	μ = 0.09 mm^{-1}
c = 10.1461 (5) Å	T = 100 (2) K
α = 99.480 (2)°	Prism, colourless
β = 97.648 (2)°	0.45 × 0.45 × 0.30 mm
γ = 106.745 (2)°	

Data collection

Nonius KappaCCD diffractometer	2441 independent reflections
φ and ω scans	1709 reflections with $I > 2\sigma(I)$
Absorption correction: none	R_{int} = 0.057
3760 measured reflections	θ_{max} = 27.0°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.045P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$(\Delta/\sigma)_{max}$ = 0.014
$wR(F^2)$ = 0.108	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
S = 1.00	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
2441 reflections	Extinction correction: *SHELXL97*
209 parameters	Extinction coefficient: 0.061 (8)
All H-atom parameters refined	

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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