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N-(4-Methylbenzyl)phthalimide

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Key indicators

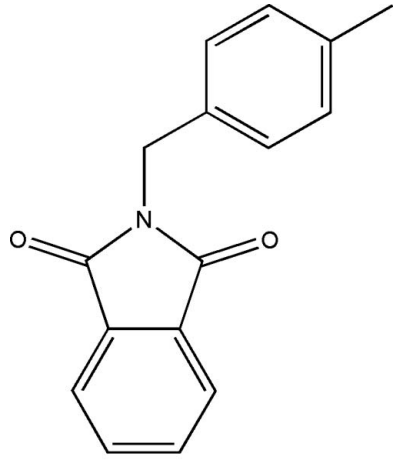
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.128
Data-to-parameter ratio = 13.3

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

The title compound, $C_{16}H_{13}NO_2$, was synthesized by *N*-alkylation of 4-methylbenzyl bromide with phthalimide. The phthalimide ring system is essentially planar and forms a dihedral angle with the tolyl ring of 69.5 (6)°.

Comment

N-Alkylated phthalimide derivatives show useful pharmaceutical properties (Chapman *et al.*, 1983; Donahoe *et al.*, 1957). In this paper, the structure of *N*-(4-methylbenzyl)-phthalimide, (I), is reported; this was synthesized by *N*-alkylation of 4-methylbenzyl bromide with phthalimide.



(I)

The phthalimide ring system (C1–C8/N1/O1/O2) is essentially planar, with a mean deviation of 0.003 Å. The dihedral angle formed between the phthalimide ring and the plane through the tolyl ring (C10–C16) is 69.5 (5)°. The molecular structure of (I) is very close to that observed for *N*-benzyl-phthalimide (Lü *et al.*, 2006; Warzecha *et al.*, 2006).

Experimental

The title compound was prepared according to the procedure of Cho *et al.* (1999). Phthalimide (1 g) was dissolved in dimethylformamide (20 ml) and treated with potassium carbonate (0.94 g) at 298 K for 30 min. To the stirred solution, 4-methylbenzyl bromide (1.25 g) was added and the mixture stirred at 298 K for a further 8 h. The resulting mixture was then poured into water (200 ml), yielding a white precipitate. The solid product was filtered off, washed with cold water and recrystallized from EtOH, giving (I) (yield: 1.67 g 97%; m.p. 393.5–394 K). Compound (I) (40 mg) was dissolved in EtOH (15 ml) and the solution was kept at 298 K for 12 d. Slow evaporation gave colourless crystals suitable for X-ray analysis.

Crystal data

$C_{16}H_{13}NO_2$
M_r = 251.27
Triclinic, $P\overline{1}$
a = 7.107 (2) Å
b = 8.521 (3) Å
c = 11.535 (4) Å
α = 102.383 (5)°
β = 100.235 (6)°
γ = 99.499 (6)°
V = 656.2 (4) Å^3
Z = 2
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
Plate, colourless
0.26 × 0.22 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.978, T_{max} = 0.993
3353 measured reflections
2303 independent reflections
1428 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.128
S = 1.04
2303 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.0787P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

All H atoms were included in the riding-model approximation, with C—H distances constrained to 0.93 (aromatic CH), 0.97 (methylene CH_2) or 0.96 Å (methyl CH_3). Isotropic displacement parameters for H atoms were fixed at U_{iso}(H) = 1.2U_{eq}(C) for aromatic CH and methylene CH_2, and at U_{iso}(H) = 1.5U_{eq}(C16) for the methyl group.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

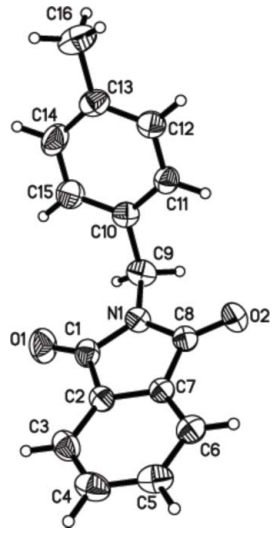


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

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