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1-(2-Methylbenzyl)-1*H*-indole-3-carbaldehyde

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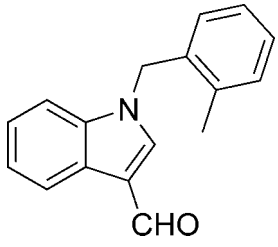
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.117; data-to-parameter ratio = 15.6.

In the title compound, $C_{17}H_{15}NO$, the benzene ring and the indole system are almost perpendicular, making a dihedral angle of 87.82 (6)°. The crystal packing is stabilized by C—H···O and π–π stacking interactions with centroid–centroid distances of 3.592 (4) Å between the pyrrole and the benzene rings in the indole systems of neighboring molecules.

Related literature

For general background to the chemistry and anti-inflammatory activity of indole aldehyde derivatives, see: Andreani *et al.* (1994).



Experimental

Crystal data

$C_{17}H_{15}NO$
M_r = 249.30
Monoclinic, $P2_1/c$
a = 10.5251 (3) Å
b = 15.4352 (5) Å
c = 8.2335 (2) Å
β = 99.214 (3)°
V = 1320.33 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.28 × 0.25 × 0.20 mm

Data collection

Agilent Xcalibur Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.981, T_{max} = 1.000
5468 measured reflections
2699 independent reflections
1928 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.117
S = 1.04
2699 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1^{i}	0.93	2.56	3.418 (2)	154

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov, 2009); software used to prepare material for publication: *OLEX2*.

We thank the Analytical and Testing Center of Sichuan University for the X-ray measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5840).

References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies Ltd, California, USA.
Andreani, A., Rambaldi, M., Locatelli, A. & Pofferi, G. (1994). *Eur. J. Med. Chem.* **29**, 903–906.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2012). E**68**, o1151 [https://doi.org/10.1107/S1600536812010306]

1-(2-Methylbenzyl)-1*H*-indole-3-carbaldehyde

Yang Wu, Wen Ren, Qiang Wang and Gu He

S1. Comment

1-(2-Methyl-benzyl)-1*H*-indole-3-carbaldehyde is of great importance owing to its wide biological properties (Andreani *et al.*, 1994). The title compound is one of the key intermediates in our synthetic investigations of antibacterial drugs. We report here its crystal structure.

In the title compound, $C_{17}H_{15}NO$, as shown in Fig 1, the benzene ring with the methyl group in *ortho* position and the indole system are almost perpendicular, making dihedral angle of 87.82 (6)°. A combination of intermolecular C-H···O and π–π packing interaction plays an important role in the connection of neighbouring molecules. The centroid-centroid distance between the pyrrole ring and the benzene ring in the indole system of the neighbouring molecule is 3.592 (4) Å (symmetry operator: -x, -y, -z).

S2. Experimental

1*H*-indole-3-carbaldehyde(14 mmol) was dissolved in dry DMF(25 ml)and treated portionwise,under stirring, with 20 mmol NaH. The mixture was stirred at room temperature for 10 min and treated with 20 mmol of 1-chloromethyl-2-methyl-benzene. After 1 h at 90°C under stirring, the mixture was poured onto ice. The resulting precipitate was collected by filtration and crystallized from ethanol with a yield of 70%. Crystals suitable for X-ray analysis were obtained by slow evaporation from a solution of dichloromethane.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C) for methyl H atoms.

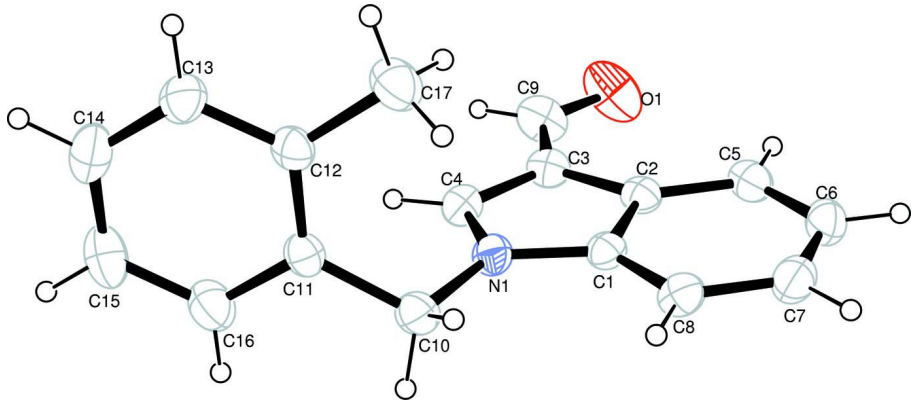


Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

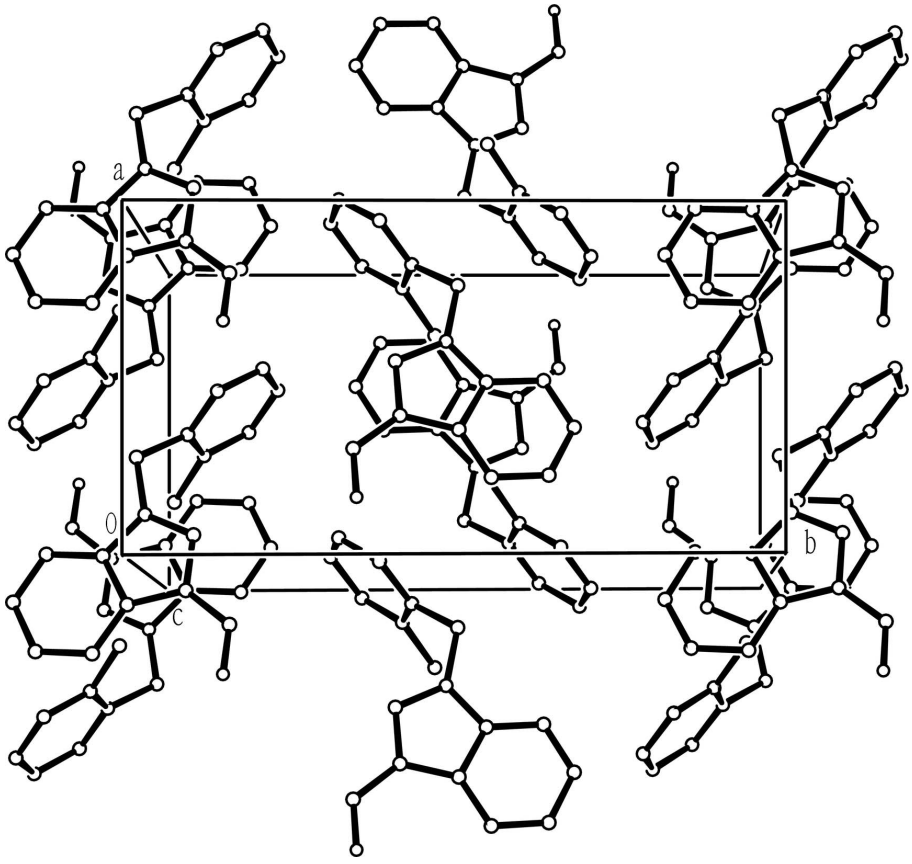


Figure 2

A packing diagram of the title compound.

1-(2-Methylbenzyl)-1*H*-indole-3-carbaldehyde

Crystal data

$C_{17}H_{15}NO$
$M_r = 249.30$
Monoclinic, $P2_1/c$
$a = 10.5251$ (3) Å
$b = 15.4352$ (5) Å
$c = 8.2335$ (2) Å
$\beta = 99.214$ (3)°
$V = 1320.33$ (7) Å^3
$Z = 4$
$F(000) = 528$
$D_x = 1.254$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å
Cell parameters from 1937 reflections
$\theta = 3.2$–29.1°
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, colorless
0.28 × 0.25 × 0.20 mm

Data collection

Agilent Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0874 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.981$, $T_{max} = 1.000$
5468 measured reflections
2699 independent reflections
1928 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 26.4°$, $\theta_{min} = 3.2°$
$h = -11 \rightarrow 13$
$k = -11 \rightarrow 19$
$l = -10 \rightarrow 4$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.117$
$S = 1.04$
2699 reflections
173 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.2065P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.02058 (15)	0.14964 (11)	−0.33644 (17)	0.0895 (5)
N1	0.21128 (12)	0.01830 (9)	0.14071 (15)	0.0439 (3)
C1	0.18887 (13)	−0.04418 (11)	0.01839 (19)	0.0404 (4)
C2	0.13295 (13)	−0.00278 (11)	−0.12762 (19)	0.0415 (4)
C3	0.12187 (14)	0.08699 (11)	−0.0886 (2)	0.0457 (4)
C4	0.17018 (15)	0.09542 (11)	0.0760 (2)	0.0475 (4)
H4	0.1739	0.1472	0.1344	0.057*
C5	0.10025 (15)	−0.05289 (13)	−0.2699 (2)	0.0506 (4)
H5	0.0639	−0.0273	−0.3687	0.061*
C6	0.12281 (16)	−0.14068 (13)	−0.2611 (2)	0.0573 (5)
H6	0.1010	−0.1744	−0.3549	0.069*
C7	0.17749 (16)	−0.17975 (12)	−0.1149 (2)	0.0567 (5)
H7	0.1910	−0.2393	−0.1126	0.068*
C8	0.21221 (15)	−0.13246 (11)	0.0266 (2)	0.0503 (4)
H8	0.2499	−0.1587	0.1242	0.060*
C9	0.06793 (18)	0.15646 (14)	−0.1918 (3)	0.0642 (5)
H9	0.0690	0.2113	−0.1449	0.077*
C10	0.26384 (17)	0.00142 (12)	0.31387 (19)	0.0536 (5)
H10A	0.3153	−0.0510	0.3210	0.064*
H10B	0.1933	−0.0082	0.3745	0.064*
C11	0.34564 (15)	0.07493 (11)	0.39236 (19)	0.0455 (4)
C12	0.46514 (15)	0.09284 (11)	0.34816 (19)	0.0448 (4)
C13	0.53745 (17)	0.15965 (12)	0.4283 (2)	0.0565 (5)
H13	0.6176	0.1721	0.4002	0.068*
C14	0.4941 (2)	0.20792 (14)	0.5479 (2)	0.0679 (6)

H14	0.5445	0.2525	0.5997	0.082*
C15	0.3765 (2)	0.19041 (15)	0.5909 (3)	0.0744 (6)
H15	0.3467	0.2228	0.6722	0.089*
C16	0.30237 (18)	0.12415 (14)	0.5125 (2)	0.0637 (5)
H16	0.2221	0.1125	0.5411	0.076*
C17	0.51550 (17)	0.04237 (15)	0.2160 (2)	0.0666 (6)
H17A	0.5075	−0.0185	0.2360	0.100*
H17B	0.6044	0.0565	0.2168	0.100*
H17C	0.4667	0.0568	0.1108	0.100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1027 (11)	0.1071 (13)	0.0562 (9)	0.0489 (10)	0.0050 (8)	0.0189 (9)
N1	0.0436 (7)	0.0468 (8)	0.0395 (7)	−0.0044 (6)	0.0014 (6)	0.0004 (7)
C1	0.0344 (8)	0.0448 (10)	0.0419 (9)	−0.0048 (7)	0.0059 (6)	−0.0003 (8)
C2	0.0307 (7)	0.0519 (10)	0.0418 (9)	−0.0009 (7)	0.0059 (6)	0.0016 (8)
C3	0.0377 (8)	0.0520 (11)	0.0471 (9)	0.0042 (7)	0.0054 (7)	0.0049 (8)
C4	0.0461 (9)	0.0446 (10)	0.0515 (10)	−0.0020 (7)	0.0070 (8)	−0.0009 (8)
C5	0.0386 (8)	0.0719 (13)	0.0404 (9)	−0.0027 (8)	0.0031 (7)	−0.0013 (9)
C6	0.0509 (10)	0.0663 (13)	0.0550 (11)	−0.0111 (9)	0.0098 (8)	−0.0169 (10)
C7	0.0570 (10)	0.0472 (11)	0.0663 (12)	−0.0060 (8)	0.0109 (9)	−0.0063 (9)
C8	0.0495 (9)	0.0482 (11)	0.0523 (10)	−0.0042 (8)	0.0052 (8)	0.0054 (9)
C9	0.0626 (12)	0.0655 (13)	0.0659 (13)	0.0204 (10)	0.0145 (10)	0.0106 (11)
C10	0.0586 (10)	0.0626 (12)	0.0381 (9)	−0.0110 (9)	0.0031 (8)	0.0043 (8)
C11	0.0486 (9)	0.0514 (10)	0.0348 (8)	−0.0002 (8)	0.0020 (7)	0.0014 (8)
C12	0.0459 (9)	0.0520 (10)	0.0345 (8)	0.0019 (8)	0.0004 (7)	0.0041 (8)
C13	0.0511 (10)	0.0644 (12)	0.0505 (10)	−0.0082 (9)	−0.0028 (8)	0.0026 (10)
C14	0.0765 (13)	0.0592 (13)	0.0622 (12)	−0.0081 (11)	−0.0073 (11)	−0.0119 (11)
C15	0.0856 (15)	0.0753 (15)	0.0612 (13)	0.0110 (12)	0.0082 (11)	−0.0251 (11)
C16	0.0579 (11)	0.0806 (15)	0.0541 (11)	0.0017 (10)	0.0133 (9)	−0.0112 (10)
C17	0.0572 (11)	0.0863 (16)	0.0584 (12)	0.0029 (10)	0.0161 (9)	−0.0093 (11)

Geometric parameters (Å, º)

O1—C9	1.220 (2)	C9—H9	0.9300
N1—C1	1.387 (2)	C10—H10A	0.9700
N1—C4	1.347 (2)	C10—H10B	0.9700
N1—C10	1.4677 (19)	C10—C11	1.506 (2)
C1—C2	1.405 (2)	C11—C12	1.392 (2)
C1—C8	1.384 (2)	C11—C16	1.381 (2)
C2—C3	1.431 (2)	C12—C13	1.385 (2)
C2—C5	1.400 (2)	C12—C17	1.502 (2)
C3—C4	1.375 (2)	C13—H13	0.9300
C3—C9	1.428 (2)	C13—C14	1.370 (3)
C4—H4	0.9300	C14—H14	0.9300
C5—H5	0.9300	C14—C15	1.367 (3)
C5—C6	1.376 (3)	C15—H15	0.9300

C6—H6	0.9300	C15—C16	1.382 (3)
C6—C7	1.386 (3)	C16—H16	0.9300
C7—H7	0.9300	C17—H17A	0.9600
C7—C8	1.374 (2)	C17—H17B	0.9600
C8—H8	0.9300	C17—H17C	0.9600

C1—N1—C10	125.15 (14)	N1—C10—H10A	109.1
C4—N1—C1	108.69 (13)	N1—C10—H10B	109.1
C4—N1—C10	126.06 (14)	N1—C10—C11	112.57 (14)
N1—C1—C2	107.72 (14)	H10A—C10—H10B	107.8
C8—C1—N1	129.84 (15)	C11—C10—H10A	109.1
C8—C1—C2	122.44 (15)	C11—C10—H10B	109.1
C1—C2—C3	106.65 (14)	C12—C11—C10	121.05 (15)
C5—C2—C1	118.56 (16)	C16—C11—C10	119.37 (16)
C5—C2—C3	134.79 (16)	C16—C11—C12	119.57 (16)
C4—C3—C2	106.38 (14)	C11—C12—C17	121.66 (15)
C4—C3—C9	124.34 (17)	C13—C12—C11	118.30 (15)
C9—C3—C2	129.24 (16)	C13—C12—C17	120.04 (16)
N1—C4—C3	110.55 (15)	C12—C13—H13	119.1
N1—C4—H4	124.7	C14—C13—C12	121.77 (17)
C3—C4—H4	124.7	C14—C13—H13	119.1
C2—C5—H5	120.6	C13—C14—H14	120.1
C6—C5—C2	118.87 (16)	C15—C14—C13	119.88 (18)
C6—C5—H5	120.6	C15—C14—H14	120.1
C5—C6—H6	119.4	C14—C15—H15	120.3
C5—C6—C7	121.23 (17)	C14—C15—C16	119.49 (18)
C7—C6—H6	119.4	C16—C15—H15	120.3
C6—C7—H7	119.3	C11—C16—C15	121.00 (18)
C8—C7—C6	121.48 (18)	C11—C16—H16	119.5
C8—C7—H7	119.3	C15—C16—H16	119.5
C1—C8—H8	121.3	C12—C17—H17A	109.5
C7—C8—C1	117.41 (16)	C12—C17—H17B	109.5
C7—C8—H8	121.3	C12—C17—H17C	109.5
O1—C9—C3	125.3 (2)	H17A—C17—H17B	109.5
O1—C9—H9	117.4	H17A—C17—H17C	109.5
C3—C9—H9	117.4	H17B—C17—H17C	109.5

N1—C1—C2—C3	−0.28 (16)	C5—C2—C3—C9	1.2 (3)
N1—C1—C2—C5	−179.55 (13)	C5—C6—C7—C8	−0.5 (3)
N1—C1—C8—C7	178.63 (15)	C6—C7—C8—C1	0.9 (2)
N1—C10—C11—C12	−69.9 (2)	C8—C1—C2—C3	179.02 (14)
N1—C10—C11—C16	111.41 (18)	C8—C1—C2—C5	−0.3 (2)
C1—N1—C4—C3	−0.86 (18)	C9—C3—C4—N1	178.46 (15)
C1—N1—C10—C11	147.04 (15)	C10—N1—C1—C2	177.28 (13)
C1—C2—C3—C4	−0.23 (16)	C10—N1—C1—C8	−1.9 (2)
C1—C2—C3—C9	−177.87 (16)	C10—N1—C4—C3	−177.41 (13)
C1—C2—C5—C6	0.6 (2)	C10—C11—C12—C13	−178.10 (15)
C2—C1—C8—C7	−0.5 (2)	C10—C11—C12—C17	2.5 (2)

C2—C3—C4—N1	0.67 (17)	C10—C11—C16—C15	178.00 (18)
C2—C3—C9—O1	0.0 (3)	C11—C12—C13—C14	−0.3 (3)
C2—C5—C6—C7	−0.3 (2)	C12—C11—C16—C15	−0.7 (3)
C3—C2—C5—C6	−178.37 (16)	C12—C13—C14—C15	0.1 (3)
C4—N1—C1—C2	0.69 (16)	C13—C14—C15—C16	−0.2 (3)
C4—N1—C1—C8	−178.54 (15)	C14—C15—C16—C11	0.5 (3)
C4—N1—C10—C11	−37.0 (2)	C16—C11—C12—C13	0.5 (2)
C4—C3—C9—O1	−177.28 (17)	C16—C11—C12—C17	−178.81 (16)
C5—C2—C3—C4	178.87 (16)	C17—C12—C13—C14	179.10 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O1^{i}	0.93	2.56	3.418 (2)	154

Symmetry code: (i) *x*, *y*, *z*+1.