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(*E*)-1-Benzyl-3-(2-nitrovinyl)-1*H*-indole

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.125
Data-to-parameter ratio = 16.8

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

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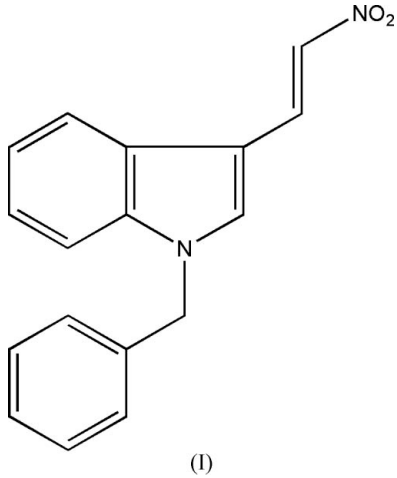
In the title molecule, $C_{17}H_{14}N_2O_2$, the indole ring system is essentially planar and makes a dihedral angle of 87.93 (3)° with the plane of the benzene ring. The nitrovinyl double bond adopts the *E* geometry.

Comment

Tryptamine is an endogenous amine found in the human brain. Serotonin and melatonin are two other essential tryptamines present in the human body. Tryptamine and its analogues can be readily synthesized by reduction of 3-(2-nitrovinyl)indoles (Shen *et al.*, 1998). The title compound is a synthetic intermediate in the synthesis of 1-benzyltryptamine, prepared by condensation of 1-benzylindole-3-carboxaldehyde with nitromethane in the presence of ammonium acetate to afford (*E*)-1-benzyl-3-(2-nitrovinyl)-1*H*-indole, (I), as a single geometrical isomer. The structure of (I) was initially identified by NMR spectroscopy. In order to confirm the double-bond geometry of the nitrovinyl group, its crystal structure determination has been carried out.



(I)

The molecular structure and atom-numbering scheme of (I) are shown in Fig. 1. Selected geometric parameters are presented in Table 1. The title compound is the *E* isomer with the C17—N2 bond in a *trans* disposition with respect to the C2—C16 bond. The indole ring system is nearly planar [with an r.m.s. deviation of all atoms of 0.009 (1) Å], and makes a dihedral angle of 87.93 (3)° with the plane of the benzene ring. The indole ring system is almost coplanar with the plane of the C16═C17 bond, as is evident from the C1—C2—C16—C17 torsion angle [173.60 (14) Å], facilitating extended conjugation between the π-electrons of the indole ring, the nitrovinyl double bond and nitro group. This extended conjugation

results in shortening of the bonds C2—C16 and C17—N2, and explains the highly coloured and crystalline nature of the title compound. In the crystal structure, molecules form centrosymmetric dimers through weak intermolecular C—H···O hydrogen bonds (Fig. 2 and Table 2).

Experimental

The title compound was prepared according to the general procedure reported by Sonar *et al.* (2005). The compound was obtained as yellow crystals.

Crystal data

$C_{17}H_{14}N_2O_2$
M_r = 278.30
Monoclinic, $P2_1/n$
a = 4.9846 (1) Å
b = 16.5617 (5) Å
c = 16.9822 (6) Å
β = 97.2220 (14)°
V = 1390.82 (7) Å^3
Z = 4
D_x = 1.329 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 150.0 (2) K
Cut needle, yellow
0.42 × 0.24 × 0.13 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.964, T_{max} = 0.989
5144 measured reflections
3189 independent reflections
2202 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.125
S = 1.03
3189 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 0.1702P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.3513 (18)	C1—C2	1.386 (2)
N2—O1	1.2308 (16)	C2—C16	1.426 (2)
N2—O2	1.2331 (16)	C16—C17	1.335 (2)
N2—C17	1.4308 (19)		
O1—N2—O2	122.61 (13)	C1—C2—C16	122.82 (14)
O1—N2—C17	120.50 (13)	N1—C9—C10	111.17 (12)
O2—N2—C17	116.88 (13)	C17—C16—C2	127.33 (14)
C1—C2—C16—C17	173.60 (14)	C2—C16—C17—N2	−179.55 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{i}	0.95	2.46	3.294 (2)	147

Symmetry code: (i) $-x+2, -y+1, -z$.

H atoms were placed in idealized positions and were constrained, with C—H = 0.99 (CH_2) and 0.95 Å (aromatic and vinyl), and U_{iso}(H) = 1.2U_{eq} of the attached C atom.

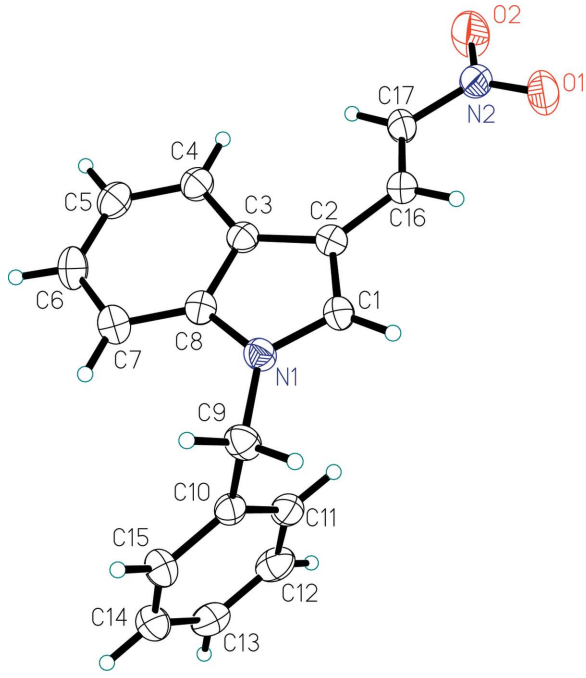


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

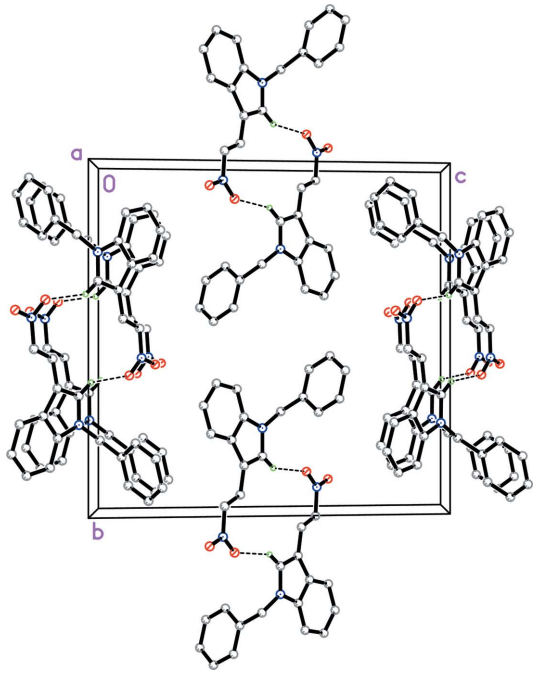


Figure 2
Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines. H atoms not involved in hydrogen bonds have been omitted.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

XP in *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97* and local procedures.

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References

Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Sheldrick (1995). *XP* in *SHELXTL/PC*. Siemens Analytical Instruments Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Shen, G., Chen, G., Cheng, Y., Xie, L. & Miao, L. (1998). *Chem. Abstr.* **130**, 13895.

Sonar, V. N., Parkin, S. & Crooks, P. A. (2005). *Acta Cryst.* C**61**, o527–o530.