

***N*-Benzyl-4-(4,4-diphenylbuta-1,3-dienyl)-*N*-ethylaniline**

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The title compound, $C_{31}H_{29}N$ or $PhCH_2(Et)NC_6H_4-CH=CHCH=CPh_2$, was synthesized by the Wittig–Horner reaction between 4-(*N*-benzyl-*N*-ethyl)aminobenzaldehyde and the phosphonate carbanion, derived from 1,1-diphenyl-3-chloropropylene and triethyl phosphite by the Arbuzov reaction. The butadiene fragment has a planar *transoid* conformation.

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Key indicators

Single-crystal X-ray study
 $T = 294\text{ K}$
 Mean $\sigma(C-C) = 0.003\text{ \AA}$
 R factor = 0.045
 wR factor = 0.128
 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>.

Comment

Organic compounds involving the butadiene group have been widely studied due to their important practical applications, most recently in connection with the manufacturing of organic light-emitting diodes (OLEDs) (Li *et al.*, 2005; Satoh *et al.*, 2003) and organic photo-conductors (OPCs) with hole-transport properties (Enokida & Hirohashi, 1991). In this paper, the structure of a new butadiene derivative, the title compound, (I), is reported. The compound was synthesized by the Wittig–Horner reaction of 4-(*N*-benzyl-*N*-ethyl)aminobenzaldehyde and the phosphonate carbanion, derived from 1,1-diphenyl-3-chloropropylene and triethyl phosphite by the Arbuzov reaction.

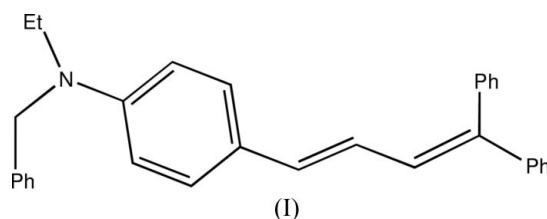
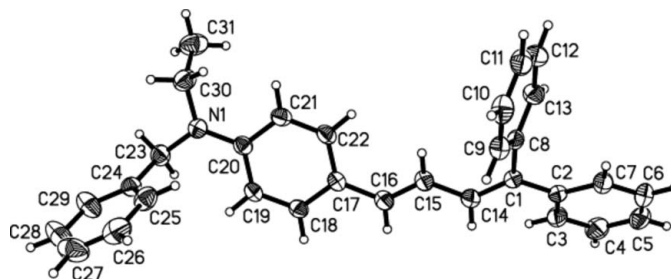


Fig. 1 shows the molecular structure of (I). The butadiene fragment $C1=C14-C15=C16$ is planar to within 0.01 \AA and has a *transoid* conformation. Both the $C1/C8/C2$ plane and the plane of the $C17-C22$ benzene ring show substantial deviations from the butadiene plane, forming dihedral angles with

**Figure 1**

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small circles of arbitrary radii.

the latter of 13.0 (2) and 17.3 (2)°, respectively. The dihedral angles formed by the plane of the C17–C22 benzene ring with the planes of the C2–C7 and C8–C13 rings are 44.4 (2) and 108.3 (2)°, respectively.

Experimental

A mixture of 1,1-diphenyl-3-chloropropylene (11.4 g, 0.05 mol) and triethyl phosphite (18.0 ml, 0.05 mol) was refluxed in xylene (50 ml) for 10 h, and then the xylene was removed *in vacuo*. After cooling, 4-(*N*-benzyl-*N*-ethyl)aminobenzaldehyde (9.6 g, 0.04 mol) and dimethylformamide (100 ml) were added to the flask containing the residue. Potassium *tert*-butoxide (4.5 g, 0.04 mol) was then added in small portions. The resulting mixture was stirred for 5 h and then poured into methanol. The precipitate was separated from the liquid by filtration, purified by silica-gel column chromatography (eluent: toluene–ethyl acetate, 2:1), recrystallized from hexane, and dried to obtain yellow crystals of (I) in 47.0% yield (m.p. 378 K). Spectroscopic analysis: MS (EIS): 416 ($M^+ + 1$); $^1\text{H NMR}$ (CDCl_3 , 500 MHz): δ 1.18 (*t*, $J = 7.5$ Hz, 3H, $-\text{CH}_3$), 3.46 (*m*, 2H, $-\text{CH}_2$), 4.50 (*s*, 2H, $-\text{CH}_2\text{Ar}$), 6.58 (*d*, 2H, $J = 9.0$ Hz, $-\text{CH}$), 6.62–6.68 (*m*, 2H, ArH), 6.84 (*d*, 1H, $J = 9.5$ Hz, $-\text{CH}$), 7.14–7.40 (*m*, 17H, ArH). Compound (I) (20 mg) was dissolved in ethyl acetate (20 ml) and the solution was left to stand at room temperature for 4 d, yielding yellow single crystals of (I) suitable for X-ray analysis.

Crystal data

$\text{C}_{31}\text{H}_{29}\text{N}$	$D_x = 1.147 \text{ Mg m}^{-3}$
$M_r = 415.55$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2899 reflections
$a = 10.4818$ (17) Å	$\theta = 2.4\text{--}23.1^\circ$
$b = 17.071$ (3) Å	$\mu = 0.07 \text{ mm}^{-1}$
$c = 13.460$ (2) Å	$T = 294$ (2) K
$\beta = 92.780$ (3)°	Block, yellow
$V = 2405.8$ (7) Å ³	$0.40 \times 0.30 \times 0.22 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART-1000 CCD area-detector diffractometer	4894 independent reflections
φ and ω scans	2709 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$R_{\text{int}} = 0.035$
$T_{\text{min}} = 0.947$, $T_{\text{max}} = 0.986$	$\theta_{\text{max}} = 26.4^\circ$
13469 measured reflections	$h = -13 \rightarrow 10$
	$k = -15 \rightarrow 21$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.2552P]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.128$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
4894 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
291 parameters	Extinction correction: <i>SHELXL97</i> (Sheldrick, 1997)
H-atom parameters constrained	Extinction coefficient: 0.0136 (13)

H atoms were positioned geometrically and refined in the riding-model approximation, with C–H = 0.93–0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, with the exception of methyl H atoms, for which $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; 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*.

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