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9-(2-Bromoethyl)-9*H*-carbazole

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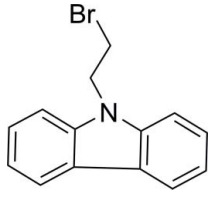
Key indicators: single-crystal X-ray study; T = 288 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.082; data-to-parameter ratio = 18.1.

In the title compound, $C_{14}H_{12}BrN$, the fused-ring system is slightly buckled as its two benzene rings are inclined to one another by 3.41 (14)°.

Related literature

For the synthesis, see: Huang *et al.* (2004). For a similar structure, see: Aravindan *et al.* (2003).



Experimental

Crystal data

$C_{14}H_{12}BrN$
M_r = 274.16
Monoclinic, $P2_1/c$
a = 5.417 (3) Å
b = 12.254 (6) Å
c = 17.505 (11) Å
β = 96.46 (3)°
V = 1154.6 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.53 mm^{-1}
T = 288 K
0.16 × 0.15 × 0.13 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.599, T_{max} = 0.657
10873 measured reflections
2630 independent reflections
2093 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.082
S = 1.02
2630 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5265).

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supplementary materials

Acta Cryst. (2012). E**68**, o2026 [doi:10.1107/S1600536812024397]

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Comment

Carozole and its derivatives are an important type of nitrogen-containing aromatic heterocyclic compounds. These special structure of carbazole compounds endow their distinct various functions as well as wide potential applications. In this paper, we report the crystal structure of the title compound.

The molecular structure of tiltle compound, $C_{14}H_{12}BrN$, as shown in Fig.1, all bond lengths and angles are in the normal ranges and are comparable with a reported compounnd (Aravindan *et al.* 2003). The dihedral angel of the two benzene rings is 3.41 (14) °. Van der Waals forces stablize the crystal structure.

Experimental

The title compound was prepared according to the literature (Huang *et al.* 2004). Single crystals suitable were prepared by slow evaporation of a dichloromethane solution of the compoundat room temperature.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 and 0.97 Å) and were included in the refinement in the riding model with U_{iso}(H) = 1.2 U_{eq}(C). The (-2 5 5) was omitted owing to bad disagreement.

Computing details

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO* (Rigaku, 1998); data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

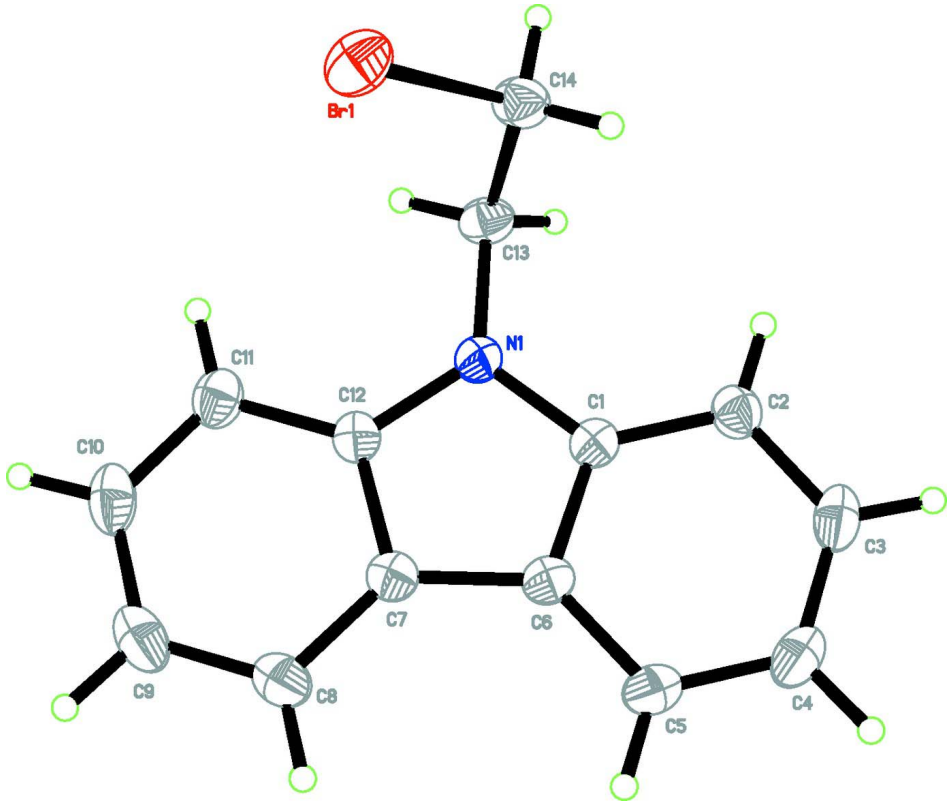

Figure 1

Molecular structure of the title compound with displacement ellipsoids drawn at the 30% probalility level.

9-(2-Bromoethyl)-9*H*-carbazole

Crystal data

$C_{14}H_{12}BrN$
$M_r = 274.16$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.417$ (3) Å
$b = 12.254$ (6) Å
$c = 17.505$ (11) Å
$\beta = 96.46$ (3)°
$V = 1154.6$ (11) Å^3
$Z = 4$
$F(000) = 552$
$D_x = 1.577$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8078 reflections
$\theta = 3.3$–27.5°
$\mu = 3.53$ mm^{-1}
$T = 288$ K
Block, colorless
0.16 × 0.15 × 0.13 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.599$, $T_{max} = 0.657$
10873 measured reflections
2630 independent reflections
2093 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -6 \rightarrow 7$
$k = -15 \rightarrow 15$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.082$
$S = 1.02$
2630 reflections
145 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
$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 0.3164P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.007$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

Special details

Experimental. (See detailed section in the paper)

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	0.25417 (5)	1.06970 (2)	0.430911 (16)	0.05611 (12)
C1	0.0265 (4)	0.88648 (17)	0.22679 (12)	0.0350 (4)
C2	−0.1470 (4)	0.94431 (18)	0.17824 (14)	0.0420 (5)
H2	−0.2717	0.9847	0.1974	0.050*
C3	−0.1273 (5)	0.9395 (2)	0.10030 (14)	0.0506 (6)
H3	−0.2424	0.9766	0.0664	0.061*
C4	0.0610 (5)	0.8802 (2)	0.07141 (14)	0.0504 (6)
H4	0.0706	0.8793	0.0187	0.060*
C5	0.2328 (4)	0.82325 (19)	0.11943 (13)	0.0446 (5)
H5	0.3591	0.7846	0.0997	0.054*
C6	0.2147 (4)	0.82425 (16)	0.19839 (12)	0.0356 (4)
C7	0.3499 (4)	0.77144 (17)	0.26390 (13)	0.0365 (5)
C8	0.5493 (4)	0.69878 (19)	0.27313 (15)	0.0473 (6)
H8	0.6248	0.6755	0.2309	0.057*
C9	0.6322 (5)	0.6623 (2)	0.34564 (18)	0.0572 (7)
H9	0.7654	0.6140	0.3522	0.069*
C10	0.5209 (5)	0.6961 (2)	0.40933 (16)	0.0546 (6)
H10	0.5813	0.6698	0.4577	0.066*
C11	0.3225 (4)	0.76790 (19)	0.40274 (14)	0.0465 (5)
H11	0.2484	0.7903	0.4455	0.056*
C12	0.2387 (4)	0.80512 (17)	0.32906 (13)	0.0357 (4)
C13	−0.1196 (4)	0.92796 (18)	0.35461 (14)	0.0417 (5)
H13A	−0.1073	0.8900	0.4035	0.050*
H13B	−0.2893	0.9207	0.3308	0.050*
C14	−0.0643 (4)	1.04724 (19)	0.36924 (15)	0.0466 (5)

H14A	−0.1951	1.0790	0.3956	0.056*
H14B	−0.0631	1.0846	0.3204	0.056*
N1	0.0445 (3)	0.87583 (15)	0.30599 (10)	0.0369 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.05008 (16)	0.06487 (19)	0.05276 (18)	−0.01404 (11)	0.00307 (12)	−0.00812 (12)
C1	0.0349 (10)	0.0342 (10)	0.0358 (11)	−0.0048 (8)	0.0038 (8)	−0.0010 (9)
C2	0.0387 (11)	0.0423 (12)	0.0441 (13)	0.0013 (9)	0.0002 (10)	0.0007 (10)
C3	0.0585 (14)	0.0479 (13)	0.0417 (14)	−0.0059 (11)	−0.0106 (11)	0.0088 (10)
C4	0.0685 (16)	0.0497 (13)	0.0322 (12)	−0.0103 (12)	0.0017 (11)	0.0014 (10)
C5	0.0533 (13)	0.0427 (12)	0.0394 (13)	−0.0039 (10)	0.0117 (10)	−0.0061 (10)
C6	0.0370 (10)	0.0337 (10)	0.0363 (11)	−0.0056 (8)	0.0055 (9)	−0.0034 (9)
C7	0.0352 (10)	0.0339 (10)	0.0401 (12)	−0.0040 (9)	0.0035 (9)	−0.0024 (9)
C8	0.0413 (11)	0.0414 (12)	0.0589 (16)	0.0033 (10)	0.0042 (11)	−0.0067 (11)
C9	0.0480 (13)	0.0421 (13)	0.078 (2)	0.0077 (11)	−0.0076 (13)	0.0035 (13)
C10	0.0585 (14)	0.0464 (13)	0.0546 (16)	−0.0029 (12)	−0.0121 (12)	0.0163 (12)
C11	0.0520 (12)	0.0456 (12)	0.0411 (13)	−0.0052 (11)	0.0011 (11)	0.0075 (10)
C12	0.0343 (10)	0.0342 (10)	0.0379 (11)	−0.0038 (8)	0.0018 (8)	0.0014 (9)
C13	0.0355 (10)	0.0477 (13)	0.0432 (13)	−0.0033 (9)	0.0105 (9)	−0.0080 (10)
C14	0.0392 (11)	0.0496 (13)	0.0507 (15)	0.0037 (10)	0.0044 (10)	−0.0084 (11)
N1	0.0376 (9)	0.0403 (9)	0.0329 (9)	0.0028 (8)	0.0048 (7)	−0.0001 (8)

Geometric parameters (Å, º)

Br1—C14	1.949 (3)	C8—C9	1.373 (4)
C1—N1	1.385 (3)	C8—H8	0.9300
C1—C2	1.389 (3)	C9—C10	1.389 (4)
C1—C6	1.408 (3)	C9—H9	0.9300
C2—C3	1.382 (4)	C10—C11	1.383 (4)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.392 (4)	C11—C12	1.395 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.372 (4)	C12—N1	1.387 (3)
C4—H4	0.9300	C13—N1	1.447 (3)
C5—C6	1.397 (3)	C13—C14	1.508 (3)
C5—H5	0.9300	C13—H13A	0.9700
C6—C7	1.443 (3)	C13—H13B	0.9700
C7—C8	1.395 (3)	C14—H14A	0.9700
C7—C12	1.410 (3)	C14—H14B	0.9700
N1—C1—C2	128.8 (2)	C10—C9—H9	119.4
N1—C1—C6	109.29 (18)	C11—C10—C9	121.7 (2)
C2—C1—C6	121.8 (2)	C11—C10—H10	119.1
C3—C2—C1	117.4 (2)	C9—C10—H10	119.1
C3—C2—H2	121.3	C10—C11—C12	117.0 (2)
C1—C2—H2	121.3	C10—C11—H11	121.5
C2—C3—C4	121.5 (2)	C12—C11—H11	121.5
C2—C3—H3	119.3	N1—C12—C11	129.1 (2)

C4—C3—H3	119.3	N1—C12—C7	109.03 (19)
C5—C4—C3	121.1 (2)	C11—C12—C7	121.9 (2)
C5—C4—H4	119.5	N1—C13—C14	113.85 (19)
C3—C4—H4	119.5	N1—C13—H13A	108.8
C4—C5—C6	118.9 (2)	C14—C13—H13A	108.8
C4—C5—H5	120.5	N1—C13—H13B	108.8
C6—C5—H5	120.5	C14—C13—H13B	108.8
C5—C6—C1	119.2 (2)	H13A—C13—H13B	107.7
C5—C6—C7	134.2 (2)	C13—C14—Br1	112.18 (16)
C1—C6—C7	106.57 (18)	C13—C14—H14A	109.2
C8—C7—C12	119.3 (2)	Br1—C14—H14A	109.2
C8—C7—C6	134.1 (2)	C13—C14—H14B	109.2
C12—C7—C6	106.66 (18)	Br1—C14—H14B	109.2
C9—C8—C7	118.9 (2)	H14A—C14—H14B	107.9
C9—C8—H8	120.5	C12—N1—C1	108.42 (17)
C7—C8—H8	120.5	C12—N1—C13	126.90 (19)
C8—C9—C10	121.2 (2)	C1—N1—C13	124.65 (18)
C8—C9—H9	119.4		