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9-Hexyl-3-iodo-9*H*-carbazole

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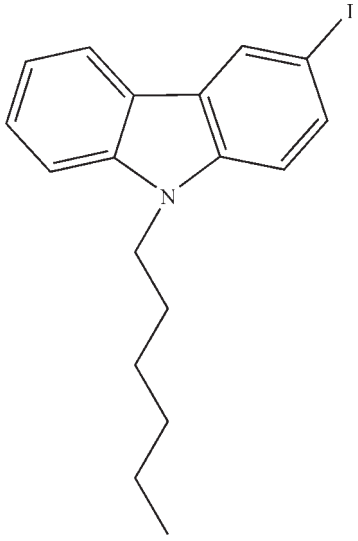
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.040; wR factor = 0.164; data-to-parameter ratio = 16.0.

In the title molecule, $C_{18}H_{20}IN$, the tricyclic carbazole system is essentially planar with the two outer rings forming a dihedral angle of 0.43 (8)°. The crystal packing exhibits no short intermolecular contacts.

Related literature

For the crystal structures of related carbazole derivatives, see: Zhou *et al.* (2007, 2008); Chen *et al.* (2009).



Experimental

Crystal data

$C_{18}H_{20}IN$
M_r = 377.25
Monoclinic, $P2_1/c$
a = 10.7105 (2) Å
b = 4.6816 (10) Å
c = 33.9661 (18) Å
β = 105.106 (8)°
V = 1644.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.94 mm^{-1}
T = 298 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.594, T_{max} = 0.698
13335 measured reflections
2904 independent reflections
2123 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.164
S = 1.14
2904 reflections
182 parameters
13 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.03 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2679).

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S1. Comment

In continuation of our study of carbazole derivatives (Zhou *et al.*, 2007, 2008) we present here the title compound, (I). In (I) (Fig. 1), the bond lengths and angles show normal values comparable with those observed in the related compounds (Zhou *et al.*, 2008; Chen *et al.*, 2009). Two outer rings form a dihedral angle of 0.43 (8) °. The crystal packing exhibits no essentially short intermolecular contacts.

S2. Experimental

A 50 ml round bottom flask was charged with 9-hexlylcarbazole (2.51 g, 10 mmol) and 10 ml e thanol. ICl (2.50 g, 15 mmol, dissolved in 4 ml ethanol) was added to the stirring solution at 343 k after 9-(hex-1-yl)-3-iodocarbazole was completely dissolved. At the end of the reaction was judged by TLC analysis after 2 h. The solution was filtered through filter paper and precipitates were obtained as a light blue solid in 89% (4.48 g) yield.

S3. Refinement

All hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 - 0.97 Å and U_{iso}(H) = 1.2-1.5U_{eq}(C).

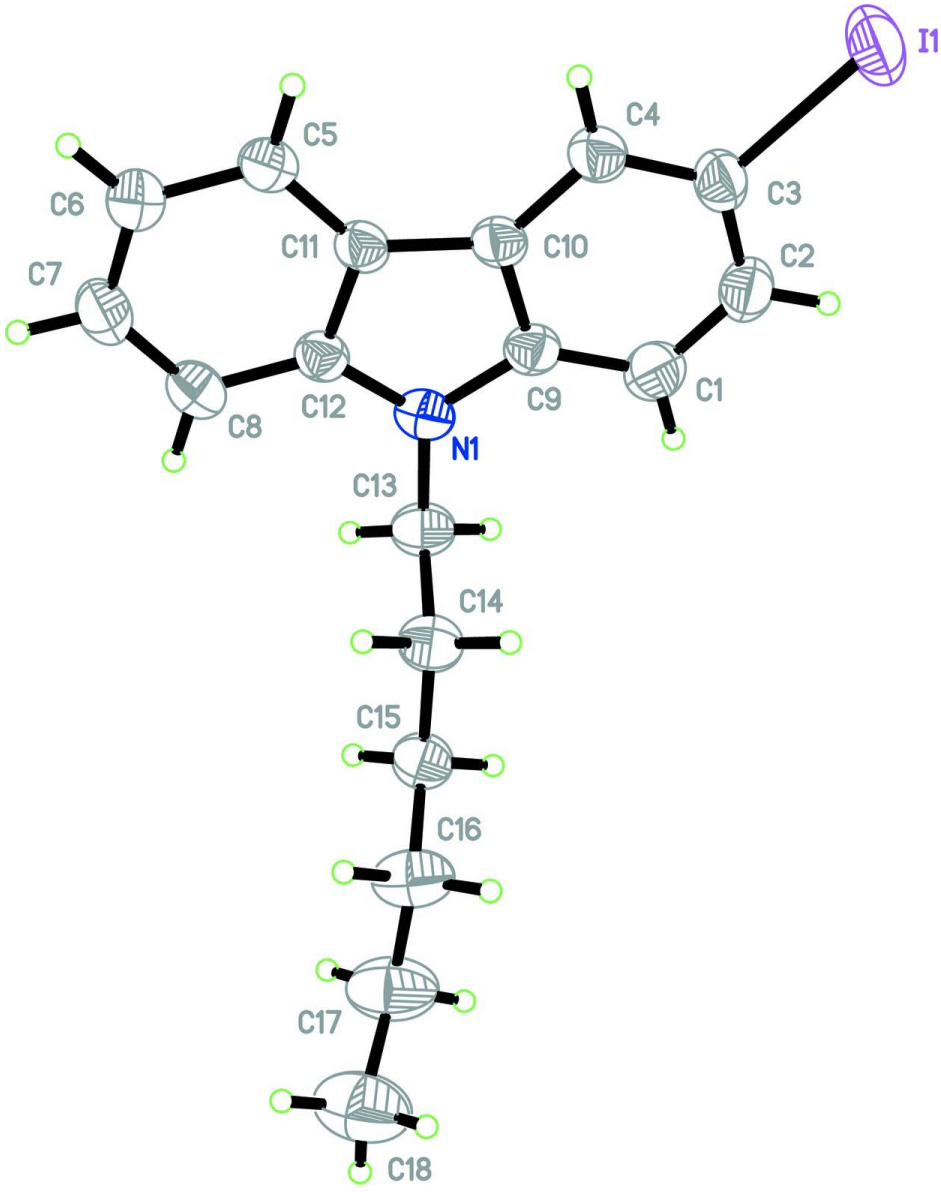

Figure 1

Molecular structure of (I) with displacement ellipsoids shown at 30% probability level.

9-Hexyl-3-iodo-9*H*-carbazole

Crystal data

$C_{18}H_{20}IN$
$M_r = 377.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.7105\ (2)$ Å
$b = 4.6816\ (10)$ Å
$c = 33.9661\ (18)$ Å
$\beta = 105.106\ (8)°$
$V = 1644.3\ (4)$ Å^3
$Z = 4$

$F(000) = 752$
$D_x = 1.524$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 4151 reflections
$\theta = 2.6–23.7°$
$\mu = 1.94$ mm^{-1}
$T = 298$ K
Bar, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.594, T_{max} = 0.698
13335 measured reflections
2904 independent reflections
2123 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −12→12
k = −5→5
l = −40→40

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.164
S = 1.14
2904 reflections
182 parameters
13 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.03 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 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}
I1	−0.28721 (3)	0.22226 (10)	0.854577 (12)	0.1016 (3)
N1	0.2490 (4)	0.7102 (7)	0.85154 (11)	0.0642 (10)
C1	0.0702 (5)	0.6986 (10)	0.88720 (15)	0.0764 (14)
H1	0.1078	0.8288	0.9075	0.092*
C2	−0.0462 (4)	0.5812 (12)	0.88584 (12)	0.0784 (13)
H2	−0.0887	0.6318	0.9054	0.094*
C3	−0.1033 (4)	0.3863 (11)	0.85567 (12)	0.0691 (11)
C4	−0.0449 (4)	0.3024 (9)	0.82657 (13)	0.0642 (11)
H4	−0.0839	0.1699	0.8068	0.077*
C5	0.1625 (4)	0.2277 (9)	0.76745 (13)	0.0642 (12)
H5	0.0931	0.1082	0.7561	0.077*
C6	0.2669 (5)	0.2482 (9)	0.75017 (15)	0.0733 (14)
H6	0.2675	0.1406	0.7272	0.088*
C7	0.3691 (4)	0.4269 (11)	0.76693 (14)	0.0752 (12)
H7	0.4373	0.4394	0.7548	0.090*
C8	0.3731 (4)	0.5878 (10)	0.80120 (12)	0.0677 (11)

H8	0.4433	0.7053	0.8125	0.081*
C9	0.1323 (4)	0.6213 (9)	0.85775 (11)	0.0588 (10)
C10	0.0761 (3)	0.4209 (9)	0.82713 (10)	0.0550 (9)
C11	0.1639 (3)	0.3892 (9)	0.80204 (10)	0.0543 (9)
C12	0.2694 (3)	0.5687 (8)	0.81814 (10)	0.0544 (9)
C13	0.3408 (4)	0.9010 (10)	0.87894 (12)	0.0705 (11)
H13A	0.2938	1.0335	0.8917	0.085*
H13B	0.3879	1.0110	0.8633	0.085*
C14	0.4357 (5)	0.7305 (8)	0.91164 (16)	0.0714 (13)
H14A	0.3878	0.6282	0.9278	0.086*
H14B	0.4777	0.5899	0.8985	0.086*
C15	0.5381 (4)	0.9110 (11)	0.93974 (13)	0.0745 (12)
H15A	0.5777	1.0328	0.9233	0.089*
H15B	0.4967	1.0340	0.9555	0.089*
C16	0.6420 (6)	0.7450 (10)	0.96843 (19)	0.096 (2)
H16A	0.6773	0.6077	0.9528	0.115*
H16B	0.6037	0.6386	0.9868	0.115*
C17	0.7505 (5)	0.9222 (13)	0.99323 (18)	0.118 (2)
H17A	0.7797	1.0512	0.9751	0.142*
H17B	0.7178	1.0378	1.0121	0.142*
C18	0.8625 (7)	0.7562 (13)	1.0167 (3)	0.144 (3)
H18A	0.9236	0.8826	1.0340	0.216*
H18B	0.9030	0.6609	0.9983	0.216*
H18C	0.8338	0.6170	1.0332	0.216*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0687 (3)	0.1321 (5)	0.1158 (4)	−0.00227 (17)	0.0452 (3)	0.0162 (2)
N1	0.054 (2)	0.068 (2)	0.065 (2)	−0.0032 (16)	0.0064 (16)	−0.0033 (15)
C1	0.075 (3)	0.086 (3)	0.066 (3)	0.011 (2)	0.015 (2)	−0.003 (2)
C2	0.073 (3)	0.104 (4)	0.063 (2)	0.018 (3)	0.027 (2)	0.009 (3)
C3	0.055 (2)	0.088 (3)	0.068 (2)	0.012 (2)	0.0223 (19)	0.017 (2)
C4	0.055 (2)	0.074 (3)	0.061 (2)	0.002 (2)	0.0105 (18)	0.0064 (19)
C5	0.052 (2)	0.073 (3)	0.064 (2)	−0.0023 (18)	0.0103 (19)	−0.0076 (18)
C6	0.066 (3)	0.086 (4)	0.069 (3)	0.001 (2)	0.021 (2)	−0.009 (2)
C7	0.058 (2)	0.087 (3)	0.086 (3)	0.003 (2)	0.029 (2)	0.008 (3)
C8	0.054 (2)	0.069 (3)	0.079 (3)	−0.006 (2)	0.0164 (19)	0.002 (2)
C9	0.055 (2)	0.064 (2)	0.054 (2)	0.009 (2)	0.0071 (17)	0.0056 (19)
C10	0.046 (2)	0.062 (2)	0.0530 (19)	0.0080 (19)	0.0067 (15)	0.0101 (18)
C11	0.0456 (19)	0.060 (2)	0.055 (2)	0.0056 (18)	0.0092 (15)	0.0071 (17)
C12	0.0479 (19)	0.057 (2)	0.0555 (19)	0.0039 (18)	0.0089 (15)	0.0050 (17)
C13	0.071 (3)	0.062 (3)	0.071 (2)	−0.005 (2)	0.006 (2)	−0.006 (2)
C14	0.071 (3)	0.062 (3)	0.077 (3)	−0.004 (2)	0.010 (2)	−0.0026 (19)
C15	0.068 (3)	0.079 (3)	0.075 (3)	−0.015 (2)	0.014 (2)	−0.009 (2)
C16	0.099 (5)	0.080 (4)	0.089 (4)	0.006 (3)	−0.009 (3)	−0.008 (2)
C17	0.118 (4)	0.090 (4)	0.121 (4)	0.005 (4)	−0.014 (3)	−0.021 (3)
C18	0.116 (6)	0.135 (6)	0.155 (6)	0.007 (4)	−0.011 (5)	−0.028 (4)

Geometric parameters (Å, º)

I1—C3	2.106 (4)	C9—C10	1.413 (6)
N1—C12	1.379 (5)	C10—C11	1.431 (5)
N1—C9	1.385 (6)	C11—C12	1.400 (5)
N1—C13	1.467 (5)	C13—C14	1.522 (6)
C1—C2	1.351 (7)	C13—H13A	0.9700
C1—C9	1.386 (7)	C13—H13B	0.9700
C1—H1	0.9300	C14—C15	1.511 (6)
C2—C3	1.389 (7)	C14—H14A	0.9700
C2—H2	0.9300	C14—H14B	0.9700
C3—C4	1.358 (6)	C15—C16	1.492 (7)
C4—C10	1.405 (6)	C15—H15A	0.9700
C4—H4	0.9300	C15—H15B	0.9700
C5—C11	1.394 (6)	C16—C17	1.496 (8)
C5—C6	1.395 (7)	C16—H16A	0.9700
C5—H5	0.9300	C16—H16B	0.9700
C6—C7	1.378 (7)	C17—C18	1.477 (7)
C6—H6	0.9300	C17—H17A	0.9700
C7—C8	1.378 (6)	C17—H17B	0.9700
C7—H7	0.9300	C18—H18A	0.9600
C8—C12	1.381 (5)	C18—H18B	0.9600
C8—H8	0.9300	C18—H18C	0.9600
C12—N1—C9	108.9 (3)	C8—C12—C11	122.1 (4)
C12—N1—C13	126.2 (4)	N1—C13—C14	110.7 (4)
C9—N1—C13	124.6 (4)	N1—C13—H13A	109.5
C2—C1—C9	118.8 (5)	C14—C13—H13A	109.5
C2—C1—H1	120.6	N1—C13—H13B	109.5
C9—C1—H1	120.6	C14—C13—H13B	109.5
C1—C2—C3	121.1 (4)	H13A—C13—H13B	108.1
C1—C2—H2	119.4	C15—C14—C13	113.9 (4)
C3—C2—H2	119.4	C15—C14—H14A	108.8
C4—C3—C2	121.9 (4)	C13—C14—H14A	108.8
C4—C3—I1	119.2 (4)	C15—C14—H14B	108.8
C2—C3—I1	118.9 (3)	C13—C14—H14B	108.8
C3—C4—C10	118.3 (4)	H14A—C14—H14B	107.7
C3—C4—H4	120.9	C16—C15—C14	114.6 (4)
C10—C4—H4	120.9	C16—C15—H15A	108.6
C11—C5—C6	118.9 (4)	C14—C15—H15A	108.6
C11—C5—H5	120.6	C16—C15—H15B	108.6
C6—C5—H5	120.6	C14—C15—H15B	108.6
C7—C6—C5	120.4 (4)	H15A—C15—H15B	107.6
C7—C6—H6	119.8	C15—C16—C17	114.6 (4)
C5—C6—H6	119.8	C15—C16—H16A	108.6
C6—C7—C8	121.8 (4)	C17—C16—H16A	108.6
C6—C7—H7	119.1	C15—C16—H16B	108.6
C8—C7—H7	119.1	C17—C16—H16B	108.6

C7—C8—C12	117.7 (4)	H16A—C16—H16B	107.6
C7—C8—H8	121.1	C18—C17—C16	114.5 (5)
C12—C8—H8	121.1	C18—C17—H17A	108.6
N1—C9—C1	130.8 (4)	C16—C17—H17A	108.6
N1—C9—C10	108.4 (4)	C18—C17—H17B	108.6
C1—C9—C10	120.8 (4)	C16—C17—H17B	108.6
C4—C10—C9	119.1 (4)	H17A—C17—H17B	107.6
C4—C10—C11	134.2 (4)	C17—C18—H18A	109.5
C9—C10—C11	106.7 (3)	C17—C18—H18B	109.5
C5—C11—C12	119.0 (4)	H18A—C18—H18B	109.5
C5—C11—C10	133.9 (4)	C17—C18—H18C	109.5
C12—C11—C10	107.1 (3)	H18A—C18—H18C	109.5
N1—C12—C8	128.9 (4)	H18B—C18—H18C	109.5
N1—C12—C11	109.0 (3)		

C9—C1—C2—C3	0.1 (7)	C6—C5—C11—C10	180.0 (4)
C1—C2—C3—C4	0.7 (7)	C4—C10—C11—C5	−0.1 (7)
C1—C2—C3—I1	−178.2 (3)	C9—C10—C11—C5	−179.3 (4)
C2—C3—C4—C10	−0.8 (6)	C4—C10—C11—C12	179.4 (4)
I1—C3—C4—C10	178.1 (3)	C9—C10—C11—C12	0.2 (4)
C11—C5—C6—C7	−0.5 (7)	C9—N1—C12—C8	−179.2 (4)
C5—C6—C7—C8	0.8 (7)	C13—N1—C12—C8	−5.2 (6)
C6—C7—C8—C12	−1.1 (7)	C9—N1—C12—C11	0.9 (4)
C12—N1—C9—C1	179.5 (4)	C13—N1—C12—C11	175.0 (4)
C13—N1—C9—C1	5.4 (7)	C7—C8—C12—N1	−178.6 (4)
C12—N1—C9—C10	−0.8 (4)	C7—C8—C12—C11	1.2 (6)
C13—N1—C9—C10	−175.0 (3)	C5—C11—C12—N1	178.9 (3)
C2—C1—C9—N1	178.8 (4)	C10—C11—C12—N1	−0.7 (4)
C2—C1—C9—C10	−0.8 (6)	C5—C11—C12—C8	−1.0 (6)
C3—C4—C10—C9	0.1 (5)	C10—C11—C12—C8	179.5 (4)
C3—C4—C10—C11	−179.1 (4)	C12—N1—C13—C14	−84.0 (5)
N1—C9—C10—C4	−179.0 (3)	C9—N1—C13—C14	89.2 (5)
C1—C9—C10—C4	0.7 (6)	N1—C13—C14—C15	176.8 (4)
N1—C9—C10—C11	0.4 (4)	C13—C14—C15—C16	−172.3 (5)
C1—C9—C10—C11	−179.9 (4)	C14—C15—C16—C17	174.0 (6)
C6—C5—C11—C12	0.6 (6)	C15—C16—C17—C18	−170.8 (7)