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2-(Carbazol-9-yl)acetic acid

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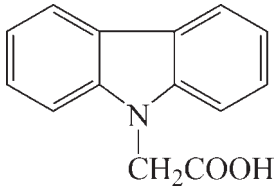
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.093; data-to-parameter ratio = 15.9.

In the title compound, $C_{14}H_{11}NO_2$, the tricyclic aromatic ring system is essentially planar [maximum deviation = 0.025 (2) Å]. The dihedral angle between the two benzene rings is 2.8 (5)°, while the carboxyl group forms a dihedral angle of 88.5 (1)° with the pyrrole ring. Intermolecular O—H···O hydrogen bonds may contribute to the overall stabilization of the crystal structure.

Related literature

For the use of the title compound in high-performance liquid chromatography, see: Jinmao *et al.* (2001). For synthesis: Xie *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{11}NO_2$ M_r = 225.24
Monoclinic, $C2/c$
a = 32.067 (19) Å
b = 5.340 (3) Å
c = 13.134 (7) Å
β = 97.756 (8)°
V = 2229 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 93 K
0.40 × 0.30 × 0.08 mm

Data collection

Rigaku SPIDER diffractometer
Absorption correction: none
8360 measured reflections
2534 independent reflections
1749 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.093
S = 1.00
2534 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···O1^{i}	0.95 (3)	1.70 (3)	2.645 (2)	171 (2)

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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: CS2123).

References

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2-(Carbazol-9-yl)acetic acid

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S1. Comment

Carbazoles are ubiquitous structural subunits of numerous naturally occurring compounds as well as synthetic materials. The title molecule (Fig. 1), is useful as an important agent for determination of alcohols by high-performance liquid chromatography with fluorimetric detection after pre-column derivatization (Jinmao *et al.*, 2001; Xie *et al.*, 2006). The crystal structure shows that the tricyclic aromatic ring system is coplanar. The dihedral angle between the two benzene rings is 2.8 (5)°. The pyrrole ring makes dihedral angles of 1.5 (5)° and 1.3 (5)° with the benzene rings, respectively. The pyrrole ring and the carboxylic acid group (O1/C14/O2) are twisted to each other by a torsion angles of 88.5 (1)°. The crystal structure may be stabilized by intermolecular O2–H2O···$O1_i$ [i= 1-x, 1-y, 1-z] hydrogen bonds.

S2. Experimental

The title compound was prepared by a method reported earlier (Xie *et al.*, 2006). The pure product (0.1 g) obtained was dissolved in 50% ethanol (10 ml). The solution was evaporated in air affording colourless platelet crystals suitable for X-ray analysis (yield: 67.2%).

S3. Refinement

Positional parameters of all the H atoms bonded to C atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded,with C—H=0.95 and 0.99 Å for aromatic and methylene and with U_{iso}(H) = 1.2U_{eq}(aromatic,methylene) parent atoms. The carboxylic H atom was taken from a differnce density map and refined.

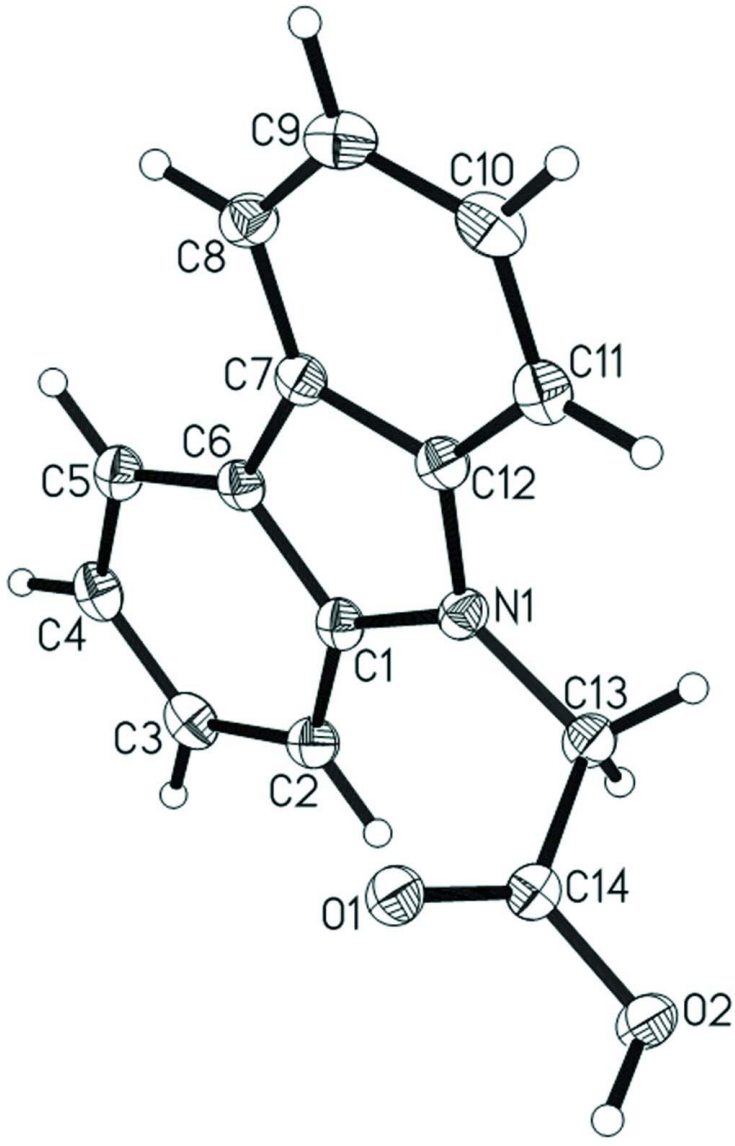

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

2-(Carbazol-9-yl)acetic acid

Crystal data

$C_{14}H_{11}NO_2$
$M_r = 225.24$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 32.067\ (19)$ Å
$b = 5.340\ (3)$ Å
$c = 13.134\ (7)$ Å
$\beta = 97.756\ (8)°$
$V = 2229\ (2)$ Å^3
$Z = 8$

$F(000) = 944$
$D_x = 1.343$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2975 reflections
$\theta = 3.1–27.5°$
$\mu = 0.09$ mm^{-1}
$T = 93$ K
Platelet, colorless
0.40 × 0.30 × 0.08 mm

Data collection

Rigaku SPIDER diffractometer
Radiation source: Rotating Anode
Graphite monochromator
ω scans
8360 measured reflections
2534 independent reflections
1749 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -41 \rightarrow 41$
$k = -6 \rightarrow 6$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.093$
$S = 1.00$
2534 reflections
159 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0136P)^2 + 0.660P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0006 (2)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.45527 (4)	0.3887 (2)	0.43806 (10)	0.0305 (3)
O2	0.48708 (4)	0.7517 (2)	0.40940 (10)	0.0322 (4)
N1	0.38917 (5)	0.4955 (3)	0.28479 (11)	0.0248 (4)
C1	0.39216 (6)	0.3113 (3)	0.21154 (13)	0.0240 (4)
C2	0.42431 (6)	0.2678 (3)	0.15246 (14)	0.0285 (5)
H2	0.4486	0.3715	0.1582	0.034*
C3	0.41955 (6)	0.0674 (3)	0.08487 (14)	0.0309 (5)
H3	0.4411	0.0330	0.0438	0.037*
C4	0.38388 (6)	−0.0852 (4)	0.07555 (14)	0.0303 (5)
H4	0.3814	−0.2204	0.0281	0.036*
C5	0.35211 (6)	−0.0411 (3)	0.13498 (14)	0.0281 (5)
H5	0.3279	−0.1456	0.1287	0.034*
C6	0.35604 (6)	0.1578 (3)	0.20388 (13)	0.0235 (4)
C7	0.33048 (6)	0.2527 (3)	0.27875 (13)	0.0245 (4)
C8	0.29237 (6)	0.1775 (4)	0.30960 (14)	0.0291 (5)
H8	0.2775	0.0374	0.2785	0.035*
C9	0.27678 (6)	0.3113 (4)	0.38653 (15)	0.0338 (5)
H9	0.2510	0.2615	0.4086	0.041*
C10	0.29835 (6)	0.5181 (4)	0.43219 (15)	0.0344 (5)
H10	0.2867	0.6077	0.4841	0.041*
C11	0.33618 (6)	0.5962 (4)	0.40406 (14)	0.0303 (5)
H11	0.3509	0.7360	0.4360	0.036*
C12	0.35197 (6)	0.4611 (3)	0.32662 (14)	0.0255 (4)
C13	0.42069 (6)	0.6818 (3)	0.31517 (14)	0.0277 (5)

H13A	0.4072	0.8275	0.3440	0.033*
H13B	0.4326	0.7395	0.2535	0.033*
C14	0.45600 (6)	0.5897 (4)	0.39346 (14)	0.0257 (4)
H2O	0.5081 (8)	0.687 (4)	0.4603 (19)	0.088 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0316 (8)	0.0297 (8)	0.0293 (8)	−0.0020 (6)	0.0000 (6)	0.0064 (6)
O2	0.0290 (8)	0.0318 (8)	0.0337 (8)	−0.0065 (7)	−0.0034 (6)	0.0074 (7)
N1	0.0252 (9)	0.0249 (9)	0.0238 (9)	−0.0024 (7)	0.0011 (7)	0.0003 (7)
C1	0.0286 (10)	0.0238 (11)	0.0187 (9)	0.0017 (8)	0.0001 (7)	0.0037 (8)
C2	0.0285 (11)	0.0308 (11)	0.0262 (10)	0.0003 (9)	0.0038 (8)	0.0068 (9)
C3	0.0373 (12)	0.0344 (12)	0.0214 (10)	0.0081 (9)	0.0057 (9)	0.0053 (9)
C4	0.0405 (12)	0.0283 (11)	0.0211 (10)	0.0068 (9)	0.0004 (9)	0.0011 (8)
C5	0.0330 (11)	0.0264 (11)	0.0235 (10)	0.0003 (9)	−0.0009 (8)	0.0019 (8)
C6	0.0262 (10)	0.0241 (11)	0.0190 (9)	0.0030 (8)	−0.0018 (7)	0.0031 (8)
C7	0.0252 (10)	0.0259 (10)	0.0210 (10)	0.0022 (8)	−0.0015 (7)	0.0040 (8)
C8	0.0261 (11)	0.0326 (12)	0.0274 (11)	−0.0014 (9)	−0.0004 (8)	0.0034 (9)
C9	0.0287 (11)	0.0460 (14)	0.0270 (11)	0.0019 (10)	0.0047 (8)	0.0056 (10)
C10	0.0354 (12)	0.0405 (13)	0.0275 (11)	0.0080 (10)	0.0043 (9)	−0.0007 (10)
C11	0.0356 (12)	0.0298 (11)	0.0240 (11)	0.0038 (9)	−0.0009 (8)	−0.0005 (9)
C12	0.0266 (10)	0.0269 (11)	0.0220 (10)	0.0015 (8)	−0.0001 (8)	0.0054 (8)
C13	0.0281 (10)	0.0275 (11)	0.0264 (10)	−0.0021 (8)	−0.0005 (8)	0.0033 (8)
C14	0.0282 (11)	0.0273 (11)	0.0221 (10)	−0.0015 (8)	0.0048 (8)	−0.0015 (8)

Geometric parameters (Å, º)

O1—C14	1.224 (2)	C5—H5	0.9500
O2—C14	1.315 (2)	C6—C7	1.454 (2)
O2—H2O	0.95 (3)	C7—C8	1.397 (2)
N1—C1	1.388 (2)	C7—C12	1.411 (2)
N1—C12	1.391 (2)	C8—C9	1.385 (3)
N1—C13	1.436 (2)	C8—H8	0.9500
C1—C2	1.391 (2)	C9—C10	1.395 (3)
C1—C6	1.412 (2)	C9—H9	0.9500
C2—C3	1.386 (2)	C10—C11	1.379 (3)
C2—H2	0.9500	C10—H10	0.9500
C3—C4	1.397 (3)	C11—C12	1.397 (2)
C3—H3	0.9500	C11—H11	0.9500
C4—C5	1.385 (3)	C13—C14	1.506 (2)
C4—H4	0.9500	C13—H13A	0.9900
C5—C6	1.390 (2)	C13—H13B	0.9900
C14—O2—H2O	109.0 (14)	C9—C8—C7	118.62 (18)
C1—N1—C12	108.85 (15)	C9—C8—H8	120.7
C1—N1—C13	124.87 (16)	C7—C8—H8	120.7
C12—N1—C13	126.21 (16)	C8—C9—C10	121.03 (19)

N1—C1—C2	129.09 (17)	C8—C9—H9	119.5
N1—C1—C6	109.17 (16)	C10—C9—H9	119.5
C2—C1—C6	121.74 (17)	C11—C10—C9	121.81 (19)
C3—C2—C1	117.42 (18)	C11—C10—H10	119.1
C3—C2—H2	121.3	C9—C10—H10	119.1
C1—C2—H2	121.3	C10—C11—C12	117.21 (18)
C2—C3—C4	121.67 (18)	C10—C11—H11	121.4
C2—C3—H3	119.2	C12—C11—H11	121.4
C4—C3—H3	119.2	N1—C12—C11	129.33 (18)
C5—C4—C3	120.51 (18)	N1—C12—C7	108.75 (17)
C5—C4—H4	119.7	C11—C12—C7	121.91 (18)
C3—C4—H4	119.7	N1—C13—C14	113.56 (15)
C4—C5—C6	119.20 (18)	N1—C13—H13A	108.9
C4—C5—H5	120.4	C14—C13—H13A	108.9
C6—C5—H5	120.4	N1—C13—H13B	108.9
C5—C6—C1	119.46 (17)	C14—C13—H13B	108.9
C5—C6—C7	134.18 (18)	H13A—C13—H13B	107.7
C1—C6—C7	106.34 (16)	O1—C14—O2	124.31 (18)
C8—C7—C12	119.41 (18)	O1—C14—C13	123.49 (17)
C8—C7—C6	133.70 (18)	O2—C14—C13	112.19 (16)
C12—C7—C6	106.88 (16)		

C12—N1—C1—C2	−177.99 (18)	C12—C7—C8—C9	0.2 (3)
C13—N1—C1—C2	−0.9 (3)	C6—C7—C8—C9	178.84 (18)
C12—N1—C1—C6	1.23 (19)	C7—C8—C9—C10	0.4 (3)
C13—N1—C1—C6	178.30 (15)	C8—C9—C10—C11	−0.9 (3)
N1—C1—C2—C3	179.41 (16)	C9—C10—C11—C12	0.8 (3)
C6—C1—C2—C3	0.3 (3)	C1—N1—C12—C11	178.33 (18)
C1—C2—C3—C4	0.3 (3)	C13—N1—C12—C11	1.3 (3)
C2—C3—C4—C5	−0.6 (3)	C1—N1—C12—C7	−0.6 (2)
C3—C4—C5—C6	0.3 (3)	C13—N1—C12—C7	−177.59 (15)
C4—C5—C6—C1	0.3 (3)	C10—C11—C12—N1	−178.94 (17)
C4—C5—C6—C7	−177.68 (18)	C10—C11—C12—C7	−0.2 (3)
N1—C1—C6—C5	−179.87 (15)	C8—C7—C12—N1	178.71 (15)
C2—C1—C6—C5	−0.6 (3)	C6—C7—C12—N1	−0.3 (2)
N1—C1—C6—C7	−1.38 (19)	C8—C7—C12—C11	−0.3 (3)
C2—C1—C6—C7	177.91 (16)	C6—C7—C12—C11	−179.28 (16)
C5—C6—C7—C8	0.4 (4)	C1—N1—C13—C14	−82.2 (2)
C1—C6—C7—C8	−177.79 (19)	C12—N1—C13—C14	94.4 (2)
C5—C6—C7—C12	179.19 (19)	N1—C13—C14—O1	−9.8 (3)
C1—C6—C7—C12	1.01 (19)	N1—C13—C14—O2	171.34 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*O*···O1^{i}	0.95 (3)	1.70 (3)	2.645 (2)	171 (2)

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