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# 3-Amino-1-(4-bromophenyl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile

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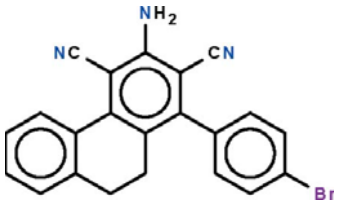
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.021; $wR$ factor = 0.056; data-to-parameter ratio = 9.0.

In the title compound, $C_{22}H_{14}BrN_3$, the fused-ring system is buckled owing to the ethylene linkage in the central ring; the two flanking aromatic rings are twisted by 25.9 (1) ° with respect to each other. The phenyl ring is twisted by 77.0 (1)° relative to the amino- and cyano-bearing aromatic ring. In the crystal, adjacent molecules are linked by two N–H···N hydrogen bonds, generating a zigzag chain along [101].

## Related literature

For two related compounds, see: Asiri *et al.* (2011*a*,*b*).




## Experimental

### Crystal data

$C_{22}H_{14}BrN_3$
$M_r$ = 400.27
Monoclinic, *Cc*
$a$ = 13.7683 (5) Å
$b$ = 16.2557 (3) Å
$c$ = 9.7945 (4) Å
$\beta$ = 127.546 (6)°
$V$ = 1738.07 (17) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 3.29 mm$^{-1}$
$T$ = 100 K
0.20 × 0.20 × 0.20 mm

### Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.559, $T_{max}$ = 0.559
2976 measured reflections
2195 independent reflections
2187 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.012

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.056
$S$ = 1.08
2195 reflections
243 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.61 e Å$^{-3}$
Absolute structure: Flack (Flack, 1983), 482 Friedel pairs
Flack parameter: −0.024 (14)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H1···N1$^{i}$ | 0.93 (3) | 2.23 (3) | 3.097 (3) | 155 (3) |
| N2—H2···N3$^{ii}$ | 0.88 (4) | 2.54 (4) | 3.307 (3) | 147 (3) |

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5646).

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