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3-Bromo-9-(4-fluorobenzyl)-9H-carbazole

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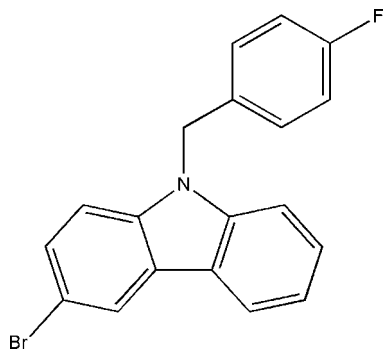
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Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å;
 R factor = 0.032; wR factor = 0.070; data-to-parameter ratio = 12.9.

The title compound, $\text{C}_{19}\text{H}_{13}\text{BrFN}$, was synthesized by *N*-alkylation of 1-chloromethyl-4-fluorobenzene with 3-bromo-9H-carbazole. The carbazole ring system is essentially planar (r.m.s. deviation of 0.024 Å for the non-H atoms) and forms a dihedral angle of 88.2 (3)° with the benzene ring.

Related literature

For a similar structure, see: Huang *et al.* (2007). For the synthetic procedure, see: Duan *et al.* (2005a,b).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{13}\text{BrFN}$
 $M_r = 354.21$
Orthorhombic, $Pna2_1$
 $a = 17.407$ (4) Å
 $b = 15.068$ (3) Å
 $c = 5.5865$ (11) Å
 $V = 1465.3$ (5) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 2.81$ mm⁻¹
 $T = 113$ K
 $0.18 \times 0.12 \times 0.08$ mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan
(*CrystalClear*; Rigaku/MSC, 2005)
 $T_{\min} = 0.632$, $T_{\max} = 0.806$
9581 measured reflections
2577 independent reflections
2294 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.070$
 $S = 0.99$
2577 reflections
199 parameters
1 restraint
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.43$ e Å⁻³
 $\Delta\rho_{\min} = -0.69$ e Å⁻³
Absolute structure: Flack (1983),
1139 Friedel pairs
Flack parameter: 0.004 (12)

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2211).

References

- Duan, X. M., Han, J., Chen, L. G., Xu, Y. J. & Li, Y. (2005a). *Fine Chem.* **22**, 39–40.
Duan, X. M., Han, J., Chen, L. G., Xu, Y. J. & Li, Y. (2005b). *Fine Chem.* **22**, 52.
Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
Huang, P.-M., Duan, X.-M. & Yang, D.-W. (2007). *Acta Cryst.* **E63**, o1264–o1265.
Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.