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# 5-[(4-Bromophenyl)methyleneimino]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1*H*-pyrazole-3-carbonitrile

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The title compound, $C_{18}H_8BrCl_2F_3N_4$, is a tricyclic imine with an overall Y shape, in which each of the three rings is planar. The pyrazole ring and the adjacent benzene ring make a dihedral angle of 88.1 (2)°. The dihedral angle between the pyrazole ring and the bromo-substituted benzene ring is 160.8 (1)°.

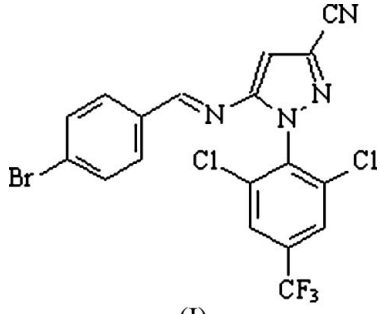
**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.012 Å
*R* factor = 0.072
*wR* factor = 0.192
Data-to-parameter ratio = 12.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

## Comment

The molecular structure of the title compound, (I), is shown in Fig. 1, with the atom-numbering scheme. It is an important starting material for the synthesis of 5-amino-3-cyano-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(trifluoromethyl)thiopyrazole, 5-amino-3-cyano-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(trifluoromethyl)sulfenylpyrazole and 5-amino-3-cyano-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(trifluoromethyl)sulfonylpyrazole, all of which are good insecticides (Hatton *et al.*, 1993). As is shown in Fig. 1, the molecule contains three planar groups, forming an overall Y shape. The pyrazole ring and the adjacent benzene ring make a dihedral angle of 88.1 (2)°. The dihedral angle between the pyrazole ring and the C1–C6 benzene ring is 160.8 (1)°. The C—F bond lengths and F—C—F angles are in normal ranges (Hassall & White, 2004).




(I)

## Experimental

According to the method of Hatton *et al.* (1993), reaction of 2,6-dichloro-4-(trifluoromethyl)aniline with a suspension of nitrosylsulfuric acid, followed by reaction with a solution of ethyl 2,3-dicyanopropionate in acetic acid, gave 5-amino-3-cyano-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]pyrazole, which was then reacted with 4-bromobenzaldehyde and hydrochloric acid in anhydrous ethanol to give the title compound, (I). This method is similar to that of many others (Zhong, Yang & Shi, 2005; Zhong, Yang, Shi *et al.*, 2005; Chen *et al.*, 2005). Colourless single crystals suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol–acetone (2:1) solution (m.p. 450–451 K).

*Crystal data*

$C_{18}H_8BrCl_2F_3N_4$
$M_r$ = 488.09
Triclinic, $P\overline{1}$
$a$ = 9.793 (3) Å
$b$ = 9.793 (3) Å
$c$ = 11.865 (3) Å
$\alpha$ = 68.361 (3)°
$\beta$ = 68.361 (3)°
$\gamma$ = 69.17°
$V$ = 950.9 (5) Å$^3$
$Z$ = 2
$D_x$ = 1.705 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 2.48 mm$^{-1}$
$T$ = 298 (2) K
Block, colourless
0.24 × 0.19 × 0.16 mm

*Data collection*

Bruker APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.587, $T_{max}$ = 0.692
4039 measured reflections
3072 independent reflections
1934 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 25.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.192
$S$ = 1.05
3072 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.088P)^2 + 0.6462P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.86 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.63 e Å$^{-3}$

All H atoms were initially located in a difference Fourier map and then placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$_{eq}$(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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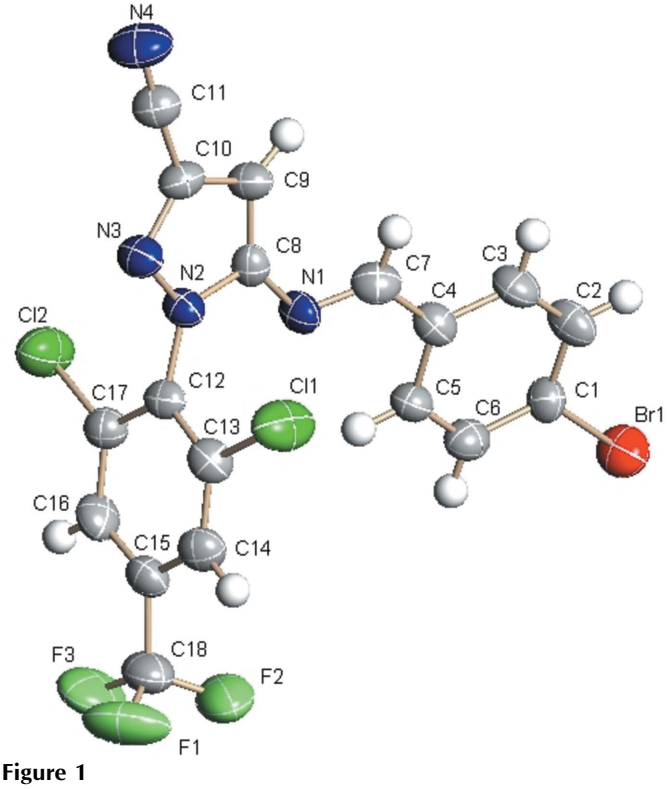


**Figure 1**
The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

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