organic compounds

(E)-1-[2,6-Dichloro-4-(trifluoromethyl)-phenyl]-5-[(dimethylamino)methylene-amino]-1H-pyrazole-4-carboxylic acid

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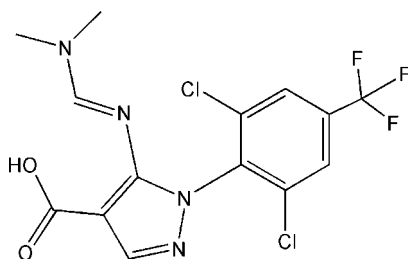
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In the crystal structure of the title compound, $C_{14}H_{11}Cl_2F_3N_4O_2$, pairs of molecules are held together by O—H$\cdots$O hydrogen bonds between the carboxyl groups, forming a centrosymmetric dimer. In the molecule, the dihedral angle between the pyrazole and benzene rings is 77.1 (3)°. The F atoms of the trifluoromethyl group are disordered over two positions with approximately equal occupancies.

Related literature

For related literature, see: Baraldi et al. (2001); Dardari et al. (2006); Hatton et al. (1993); Jin et al. (2004); Li et al. (2006); Smith et al. (2001); Zhong et al. (2006).

Experimental

Crystal data

$C_{14}H_{11}Cl_2F_3N_4O_2$	Monoclinic, $C2/c$
$M_r = 395.17$	$a = 16.4987 (15)$ Å
	$b = 17.5642 (16)$ Å
	$c = 11.8035 (11)$ Å
	$\beta = 95.626 (2)°$
	$V = 3404.0 (5)$ Å^3
	$Z = 8$
Mo $K\alpha$ radiation	
$\mu = 0.43$ mm^{-1}	
$T = 273 (2)$ K	
$0.33 \times 0.24 \times 0.17$ mm	

Data collection

Bruker APEX area-detector diffractometer	8810 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000) $T_{min} = 0.872$, $T_{max} = 0.931$	3000 independent reflections
	2507 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.079$	3 restraints
$wR(F^2) = 0.192$	H-atom parameters constrained
$S = 1.13$	$\Delta\rho_{max} = 0.67$ e Å^{-3}
3000 reflections	$\Delta\rho_{min} = -0.43$ e Å^{-3}
233 parameters	

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

D—H$\cdots$A	D—H	H$\cdots$A	$D\cdots$A	D—H$\cdots$A
O2—H2$\cdots$O1[i]	0.82	1.86	2.668 (4)	169

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); 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, 2000); software used to prepare material for publication: SHELXTL.

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supplementary materials

(*E*)-1-[2,6-Dichloro-4-(trifluoromethyl)phenyl]-5-[(dimethylamino)methyleneamino]-1*H*-pyrazole-4-carboxylic acid

D.-M. Xie, Z. Shu, L. Shen, Z.-W. Ding and Z.-M. Jin

Comment

Various biological activities of pyrazole derivatives, such as antitumor (Baraldi *et al.*, 2001), anti-inflammatory (Smith *et al.*, 2001) and antimicrobial activities (Hatton *et al.*, 1993), have been indicated by a large number of reports. In addition, they have been used as ligands to investigate the relationship between the structure and the activity of the active site of metalloproteins (Dardari *et al.*, 2006). For possible biological activity, the title compound was synthesized in our laboratory.

As shown in Fig. 1, the molecule has an overall *L* shape. The dihedral angel between the pyrazole ring and the benzene ring is 77.1 (3)°. The C—N bond lengths in the pyrazole ring range from 1.310 (5) to 1.361 (5) Å, which are shorter than a C—N single bond length of 1.443 Å, but longer than a typical C═N bond length of 1.269 Å (Jin *et al.*, 2004), indicating the electron delocalization. Most bond lengths and angles in *N*-phenylpyrazole group are similar with the analogous molecules (Li *et al.*, 2006; Zhong *et al.*, 2006). Three disordered F atoms are observed in the trifluoromethyl group.

An O—H⋯O intermolecular interaction, which forms a dimeric motif typical for carboxylic acid, is an essential force in the crystal form (Fig. 2).

Experimental

The title compound was synthesized according to the method of Hatton *et al.* (1993) and single crystals were obtained by slow evaporation of an acetone solution.

Refinement

Three F atoms were split into approximately equal components with occupancies of 0.443 (18) for F1', F2' and F3' atoms, and 0.557 (18) for F1, F2 and F3 atoms. All H atoms were placed in calculated positions (O—H = 0.82 and C—H = 0.93 − 0.96 Å), and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2–1.5 U_{eq}(C,O)$. The distances of C1—F1' and C1—F1 are restrained to be equal within a standard uncertainty of 0.01 Å. The same restraints have been applied for C1—F2' and C1—F2, and for C1—F3' and C1—F3.
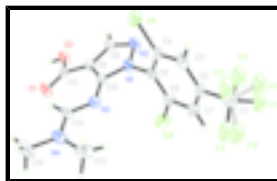
Figures

Fig. 1. The molecular structure of the title compound with atom labels, showing 30% probability displacement ellipsoids.
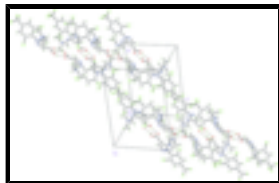
Fig. 2. A packing diagram, viewed approximately along the *b* axis. Hydrogen bonds are indicated by dashed lines.

(*E*)-1-[2,6-Dichloro-4-(trifluoromethyl)phenyl]-5-\ [(dimethylamino)methyleneamino]-1*H*-pyrazole-4-carboxylic acid

Crystal data

$C_{14}H_{11}Cl_2F_3N_4O_2$	$F_{000} = 1600$
$M_r = 395.17$	$D_x = 1.542$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 2395 reflections
$a = 16.4987$ (15) Å	$\theta = 2.3–24.0º$
$b = 17.5642$ (16) Å	$\mu = 0.43$ mm^{-1}
$c = 11.8035$ (11) Å	$T = 273$ (2) K
$\beta = 95.626$ (2)º	Block, colorless
$V = 3404.0$ (5) Å^3	$0.33 \times 0.24 \times 0.17$ mm
$Z = 8$	

Data collection

Bruker APEX area-detector diffractometer	3000 independent reflections
Radiation source: fine-focus sealed tube	2507 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 273(2)$ K	$\theta_{max} = 25.0º$
φ and ω scan	$\theta_{min} = 1.7º$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$h = -18\rightarrow19$
$T_{min} = 0.872$, $T_{max} = 0.931$	$k = -20\rightarrow17$
8810 measured reflections	$l = -14\rightarrow13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.079$	H-atom parameters constrained
$wR(F^2) = 0.192$	$w = 1/[\sigma^2(F_o^2) + (0.0731P)^2 + 12.0677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} < 0.001$
3000 reflections	$\Delta\rho_{max} = 0.67$ e Å^{-3}
233 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}

3 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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 ($\mathring{A}^2$)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.14889 (7)	0.32685 (8)	−0.03790 (10)	0.0589 (4)	
Cl2	0.36248 (9)	0.41783 (9)	0.30881 (12)	0.0749 (5)	
F1	0.5128 (6)	0.3254 (7)	−0.0513 (10)	0.095 (3)	0.443 (18)
F2	0.4306 (6)	0.3471 (8)	−0.1977 (7)	0.095 (3)	0.443 (18)
F3	0.4852 (7)	0.4397 (5)	−0.0970 (11)	0.095 (3)	0.443 (18)
F1'	0.4841 (6)	0.3031 (4)	−0.0965 (10)	0.099 (3)	0.557 (18)
F2'	0.4231 (4)	0.3860 (7)	−0.2011 (6)	0.099 (3)	0.557 (18)
F3'	0.5109 (5)	0.4214 (5)	−0.0690 (9)	0.099 (3)	0.557 (18)
O1	0.0486 (2)	0.51875 (17)	0.3874 (3)	0.0524 (8)	
O2	0.0227 (2)	0.40406 (17)	0.4549 (3)	0.0531 (8)	
H2	−0.0039	0.4292	0.4966	0.080*	
N1	0.1993 (2)	0.37409 (19)	0.2005 (3)	0.0414 (8)	
N2	0.1734 (2)	0.30728 (19)	0.2448 (3)	0.0479 (9)	
N3	0.1879 (2)	0.50406 (19)	0.1939 (3)	0.0413 (8)	
N4	0.1740 (3)	0.6305 (2)	0.1563 (3)	0.0559 (10)	
C1	0.4523 (4)	0.3719 (4)	−0.0896 (5)	0.0700 (16)	
C2	0.3847 (3)	0.3741 (3)	−0.0164 (4)	0.0533 (12)	
C3	0.3074 (3)	0.3531 (3)	−0.0585 (4)	0.0514 (12)	
H3	0.2963	0.3388	−0.1343	0.062*	
C4	0.2465 (3)	0.3536 (2)	0.0134 (4)	0.0426 (10)	
C5	0.2623 (3)	0.3735 (2)	0.1267 (4)	0.0410 (10)	
C6	0.3407 (3)	0.3938 (3)	0.1672 (4)	0.0498 (11)	
C7	0.4024 (3)	0.3947 (3)	0.0958 (5)	0.0577 (13)	
H7	0.4550	0.4090	0.1232	0.069*	
C8	0.1186 (3)	0.3302 (2)	0.3104 (4)	0.0449 (11)	
H8	0.0893	0.2970	0.3523	0.054*	
C9	0.1080 (2)	0.4092 (2)	0.3116 (3)	0.0371 (9)	
C10	0.1622 (2)	0.4376 (2)	0.2361 (3)	0.0352 (9)	
C11	0.0578 (2)	0.4502 (2)	0.3855 (3)	0.0371 (9)	
C12	0.1481 (3)	0.5665 (2)	0.1987 (3)	0.0421 (10)	

H12	0.0998	0.5666	0.2331	0.050*
C13	0.2477 (4)	0.6321 (3)	0.0987 (5)	0.0806 (18)
H13A	0.2814	0.5894	0.1230	0.121*
H13B	0.2768	0.6785	0.1172	0.121*
H13C	0.2337	0.6294	0.0180	0.121*
C14	0.1268 (4)	0.7004 (3)	0.1562 (5)	0.0836 (19)
H14A	0.1114	0.7159	0.0791	0.125*
H14B	0.1592	0.7396	0.1951	0.125*
H14C	0.0788	0.6919	0.1943	0.125*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0473 (7)	0.0747 (9)	0.0558 (7)	0.0095 (6)	0.0110 (5)	0.0027 (6)
Cl2	0.0635 (8)	0.1047 (12)	0.0589 (8)	−0.0124 (7)	0.0179 (6)	−0.0245 (7)
F1	0.080 (4)	0.094 (5)	0.123 (5)	0.007 (3)	0.069 (4)	−0.008 (3)
F2	0.080 (4)	0.094 (5)	0.123 (5)	0.007 (3)	0.069 (4)	−0.008 (3)
F3	0.080 (4)	0.094 (5)	0.123 (5)	0.007 (3)	0.069 (4)	−0.008 (3)
F1'	0.079 (3)	0.101 (4)	0.128 (5)	0.004 (2)	0.072 (3)	−0.013 (3)
F2'	0.079 (3)	0.101 (4)	0.128 (5)	0.004 (2)	0.072 (3)	−0.013 (3)
F3'	0.079 (3)	0.101 (4)	0.128 (5)	0.004 (2)	0.072 (3)	−0.013 (3)
O1	0.068 (2)	0.0393 (18)	0.0565 (19)	0.0054 (15)	0.0407 (16)	−0.0021 (14)
O2	0.066 (2)	0.0448 (17)	0.055 (2)	0.0022 (15)	0.0413 (16)	−0.0003 (15)
N1	0.047 (2)	0.0362 (19)	0.045 (2)	0.0019 (15)	0.0259 (16)	−0.0005 (15)
N2	0.057 (2)	0.036 (2)	0.056 (2)	0.0019 (17)	0.0310 (19)	0.0012 (16)
N3	0.046 (2)	0.038 (2)	0.043 (2)	−0.0018 (16)	0.0222 (16)	0.0004 (15)
N4	0.079 (3)	0.040 (2)	0.051 (2)	−0.0044 (19)	0.014 (2)	0.0047 (17)
C1	0.075 (4)	0.070 (4)	0.072 (4)	0.001 (3)	0.046 (3)	−0.006 (3)
C2	0.053 (3)	0.049 (3)	0.064 (3)	0.004 (2)	0.032 (2)	0.000 (2)
C3	0.062 (3)	0.053 (3)	0.044 (3)	0.012 (2)	0.027 (2)	0.002 (2)
C4	0.044 (2)	0.038 (2)	0.049 (3)	0.0120 (18)	0.0189 (19)	0.0025 (19)
C5	0.043 (2)	0.035 (2)	0.049 (3)	0.0066 (18)	0.0245 (19)	−0.0009 (19)
C6	0.049 (3)	0.051 (3)	0.053 (3)	0.000 (2)	0.020 (2)	−0.009 (2)
C7	0.044 (3)	0.060 (3)	0.073 (4)	−0.004 (2)	0.027 (2)	−0.007 (3)
C8	0.053 (3)	0.042 (2)	0.045 (2)	−0.0051 (19)	0.026 (2)	0.0027 (19)
C9	0.038 (2)	0.041 (2)	0.035 (2)	−0.0017 (17)	0.0148 (17)	−0.0039 (17)
C10	0.034 (2)	0.037 (2)	0.036 (2)	−0.0002 (17)	0.0120 (16)	−0.0047 (17)
C11	0.031 (2)	0.046 (3)	0.036 (2)	−0.0026 (17)	0.0137 (16)	−0.0016 (18)
C12	0.055 (3)	0.037 (2)	0.036 (2)	0.000 (2)	0.0121 (19)	−0.0035 (18)
C13	0.091 (4)	0.073 (4)	0.082 (4)	−0.026 (3)	0.030 (3)	0.017 (3)
C14	0.138 (6)	0.040 (3)	0.073 (4)	0.013 (3)	0.013 (4)	0.005 (3)

Geometric parameters (Å, °)

Cl1—C4	1.729 (5)	C1—C2	1.477 (7)
Cl2—C6	1.728 (5)	C2—C3	1.374 (7)
F1—C1	1.333 (9)	C2—C7	1.377 (7)
F2—C1	1.362 (9)	C3—C4	1.377 (6)
F3—C1	1.315 (9)	C3—H3	0.9300

F1'—C1	1.322 (8)	C4—C5	1.382 (6)
F2'—C1	1.379 (9)	C5—C6	1.380 (6)
F3'—C1	1.306 (8)	C6—C7	1.384 (6)
O1—C11	1.214 (5)	C7—H7	0.9300
O2—C11	1.325 (5)	C8—C9	1.399 (6)
O2—H2	0.8200	C8—H8	0.9300
N1—C10	1.359 (5)	C9—C10	1.413 (5)
N1—N2	1.370 (5)	C9—C11	1.452 (5)
N1—C5	1.421 (5)	C12—H12	0.9300
N2—C8	1.310 (5)	C13—H13A	0.9600
N3—C12	1.282 (5)	C13—H13B	0.9600
N3—C10	1.353 (5)	C13—H13C	0.9600
N4—C12	1.318 (5)	C14—H14A	0.9600
N4—C13	1.451 (7)	C14—H14B	0.9600
N4—C14	1.453 (7)	C14—H14C	0.9600
C11—O2—H2	109.5	C5—C6—C7	120.8 (4)
C10—N1—N2	114.7 (3)	C5—C6—Cl2	119.8 (3)
C10—N1—C5	125.0 (3)	C7—C6—Cl2	119.4 (4)
N2—N1—C5	120.2 (3)	C2—C7—C6	118.9 (5)
C8—N2—N1	102.8 (3)	C2—C7—H7	120.6
C12—N3—C10	122.8 (3)	C6—C7—H7	120.6
C12—N4—C13	120.7 (4)	N2—C8—C9	113.8 (4)
C12—N4—C14	121.9 (5)	N2—C8—H8	123.1
C13—N4—C14	117.2 (4)	C9—C8—H8	123.1
F3'—C1—F1'	109.2 (6)	C8—C9—C10	104.9 (3)
F3—C1—F1	106.1 (7)	C8—C9—C11	125.2 (4)
F3—C1—F2	107.4 (8)	C10—C9—C11	129.6 (4)
F1—C1—F2	104.0 (7)	N3—C10—N1	115.3 (3)
F3'—C1—F2'	103.9 (7)	N3—C10—C9	141.0 (4)
F1'—C1—F2'	102.1 (6)	N1—C10—C9	103.7 (3)
F3'—C1—C2	117.4 (6)	O1—C11—O2	122.2 (3)
F3—C1—C2	110.7 (6)	O1—C11—C9	125.6 (4)
F1'—C1—C2	112.8 (5)	O2—C11—C9	112.2 (4)
F1—C1—C2	113.7 (6)	N3—C12—N4	121.8 (4)
F2—C1—C2	114.3 (6)	N3—C12—H12	119.1
F2'—C1—C2	109.9 (6)	N4—C12—H12	119.1
C3—C2—C7	121.4 (4)	N4—C13—H13A	109.5
C3—C2—C1	120.6 (5)	N4—C13—H13B	109.5
C7—C2—C1	118.0 (5)	H13A—C13—H13B	109.5
C2—C3—C4	118.9 (4)	N4—C13—H13C	109.5
C2—C3—H3	120.6	H13A—C13—H13C	109.5
C4—C3—H3	120.6	H13B—C13—H13C	109.5
C3—C4—C5	121.2 (4)	N4—C14—H14A	109.5
C3—C4—Cl1	119.5 (4)	N4—C14—H14B	109.5
C5—C4—Cl1	119.3 (3)	H14A—C14—H14B	109.5
C6—C5—C4	118.8 (4)	N4—C14—H14C	109.5
C6—C5—N1	120.2 (4)	H14A—C14—H14C	109.5
C4—C5—N1	121.0 (4)	H14B—C14—H14C	109.5

C10—N1—N2—C8	−0.3 (5)	N1—C5—C6—C7	−178.9 (4)
C5—N1—N2—C8	177.7 (4)	C4—C5—C6—Cl2	−179.2 (3)
F3'—C1—C2—C3	149.3 (8)	N1—C5—C6—Cl2	1.5 (6)
F3—C1—C2—C3	120.9 (9)	C3—C2—C7—C6	0.2 (7)
F1'—C1—C2—C3	−82.4 (9)	C1—C2—C7—C6	−177.0 (5)
F1—C1—C2—C3	−119.8 (9)	C5—C6—C7—C2	−0.8 (7)
F2—C1—C2—C3	−0.6 (11)	Cl2—C6—C7—C2	178.8 (4)
F2'—C1—C2—C3	30.8 (9)	N1—N2—C8—C9	−0.5 (5)
F3'—C1—C2—C7	−33.5 (10)	N2—C8—C9—C10	1.0 (5)
F3—C1—C2—C7	−61.8 (10)	N2—C8—C9—C11	−173.2 (4)
F1'—C1—C2—C7	94.9 (9)	C12—N3—C10—N1	164.6 (4)
F1—C1—C2—C7	57.5 (10)	C12—N3—C10—C9	−17.8 (8)
F2—C1—C2—C7	176.7 (9)	N2—N1—C10—N3	179.3 (4)
F2'—C1—C2—C7	−151.9 (7)	C5—N1—C10—N3	1.5 (6)
C7—C2—C3—C4	0.7 (7)	N2—N1—C10—C9	0.9 (5)
C1—C2—C3—C4	177.9 (5)	C5—N1—C10—C9	−177.0 (4)
C2—C3—C4—C5	−1.1 (7)	C8—C9—C10—N3	−178.8 (5)
C2—C3—C4—Cl1	−179.6 (4)	C11—C9—C10—N3	−5.0 (9)
C3—C4—C5—C6	0.6 (6)	C8—C9—C10—N1	−1.1 (4)
Cl1—C4—C5—C6	179.1 (3)	C11—C9—C10—N1	172.8 (4)
C3—C4—C5—N1	179.9 (4)	C8—C9—C11—O1	179.7 (4)
Cl1—C4—C5—N1	−1.6 (5)	C10—C9—C11—O1	7.0 (7)
C10—N1—C5—C6	75.9 (6)	C8—C9—C11—O2	0.8 (6)
N2—N1—C5—C6	−101.8 (5)	C10—C9—C11—O2	−171.9 (4)
C10—N1—C5—C4	−103.4 (5)	C10—N3—C12—N4	−179.5 (4)
N2—N1—C5—C4	78.9 (5)	C13—N4—C12—N3	2.0 (7)
C4—C5—C6—C7	0.4 (7)	C14—N4—C12—N3	176.6 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1[i]	0.82	1.86	2.668 (4)	169

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

Fig. 1

Fig. 2