Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*Z*)-3-[(2-Fluoroanilino)carbonyl]prop-2-enoic acid

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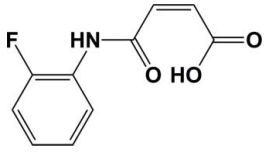
Received 20 December 2010; accepted 8 January 2011

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.121; data-to-parameter ratio = 8.1.

In the title molecule, $C_{10}H_8FNO_3$, the dihedral angle between the fluorophenyl group and the essentially planar [within 0.064 (3) Å] COC=CCOOH unit, which has a Z configuration, is 19.99 (14)°. There is an intramolecular O—H···O bond in the molecule involving the acid –OH group and the adjacent carbonyl O atom. In the crystal, intermolecular N—H···O bonds lead to the formation of polymer chains propagating along [011].

Related literature

For the use of carboxylic acids containing N atoms as antibiotics, see: Gould *et al.* (1980). For the biological properties of compounds containing keto, ester, imide and carboxylc acid groups, see: Chen & Njoroge (2009); Shen & Walford (1972; 1980). For the structure of 3-[(4-bromoanilino)carbonyl]prop-2-enoic acid, see Parvez, Shahid *et al.* (2004). For the structure of 3-[(2,4,6-tricholoroanilino)carbonyl]prop-2-enoic acid, see Parvez, Shahzadi *et al.*(2004).



Experimental

Crystal data

$C_{10}H_8FNO_3$
M_r = 209.17
Orthorhombic, $Pna2_1$
a = 20.282 (2) Å
b = 3.8025 (4) Å
c = 11.8183 (8) Å
V = 911.45 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 299 K
0.57 × 0.21 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
7575 measured reflections
1075 independent reflections
799 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.121
S = 1.09
1075 reflections
132 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O1	0.92 (8)	1.60 (8)	2.506 (4)	170 (7)
N1—H1A···O2^{i}	0.83 (5)	2.10 (5)	2.929 (5)	175 (4)

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2007); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

SA is thankful to Quaid-i-Azam University, Islamabad, Pakistan, for financial support. The Swedish Research Council (VR) is acknowledged for providing funding for the single-crystal diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2241).

References

Brandenburg, K. (2007). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Chen, K. X. & Njoroge, F. G. (2009). *Curr. Opin. Invest. Drugs*, **10**, 821–837.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Gould, S. J., Chang, C. C., Darling, D. S., Roberts, J. D. & Squillacote, M. (1980). *J. Am. Chem. Soc.* **102**, 1707–1712.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Parvez, M., Shahid, K., Shahzadi, S. & Ali, S. (2004). *Acta Cryst.* E**60**, o2079–o2081.
Parvez, M., Shahzadi, S., Shahid, K. & Ali, S. (2004). *Acta Cryst.* E**60**, o2082–o2084.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shen, T.-Y. & Walford, G. L. (1972). US Patent 3 655 692.
Shen, T.-Y. & Walford, G. L. (1980). US Patent 3 547 948.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, o393 [doi:10.1107/S1600536811001152]

(*Z*)-3-[(2-Fluoroanilino)carbonyl]prop-2-enoic acid

Farooq Ali Shah, Saqib Ali, Saira Shahzadi, Sajjad Ahmad and Andreas Fischer

S1. Comment

Carboxylic acids are good reducing agents and applied as an antioxidant agent and a precursor for the prevention of cancer. Carboxylic acids are used for therapeutic purposes and for other biological applications as well. Those carboxylic acids which contain N atoms are widely used as antibiotics (Gould *et al.*, 1980). Compounds containing NH and carboxyl groups are of great interest for the synthesis of drugs due to their coordination to biological systems. Compounds containing keto, ester and imide are good anti-HCV agents (Chen *et al.*, 2009). Carboxylic acids are also used as anti-inflammatories (Shen & Walford, 1980) and enzymetic inhibitors (Shen & Walford, 1972). We therefore used maleic anhydride to synthesize the title compound, by condensation with 2-fluoroaniline.

The molecular structure of the title compound is illustrated in Fig. 1. The bond distances and angles are close to those observed in simlar compounds; 3-[(4-bromoanilino)carbonyl]prop-2-enoic acid (Parvez, Shahid *et al.*, 2004) and 3-[(2,4,6-Tricholoroanilino)carbonyl]prop-2-enoic acid (Parvez, Shahzadi *et al.*, 2004). In the molecule there is an intramolecular O—H···O hydrogen bond involving the acid OH group and the adjacent carbonyl O-atom (Table 1). The COC=CCOOH moiety is essentially planar [atoms O1,C7—C10, O2,O3 planar to within 0.064 (3) Å], and has a *Z* configuration. It makes a dihedral angle of 19.99 (14) Å with the phenyl ring.

In the crystal there are intermolecular N–H···.O hydrogen bonds connecting symmetry related molecules yielding chains propagating along [011] (Table 1 and Fig. 2).

S2. Experimental

A solution of maleic anhydride (5 g, 1 mmol) in (300 ml glacial acetic acid) was added to a solution of 2-fluoroaniline (5 ml, 1 mmol) (150 ml glacial acetic acid) in 500 ml beaker at room temperature and the mixture was stirred in fuming hood at room temperature overnight. The light yellow precipitates formed were filtered off, washed with cold distilled H_2O (200 ml) and air dried. The yellow crystals, suitable for X-ray diffraction analysis, were obtained by recrystallization in acetone:n-hexane (1:1).

S3. Refinement

In the final cycles of refinement, in the absence of significant anomalous scattering effects, 719 Friedel pairs were merged and Δf '' set to zero. The OH and NH H-atoms were located from a difference Fourier map and were freely refined: O3—H3B = 0.92 (8) Å, N1—H1A = 0.83 (5) Å. The C-bound H-atoms were included in calculated positions and treated as riding atoms: C—H = 0.93 Å with U_{iso}(H) = 1.2U_{eq}(parent C-atom).

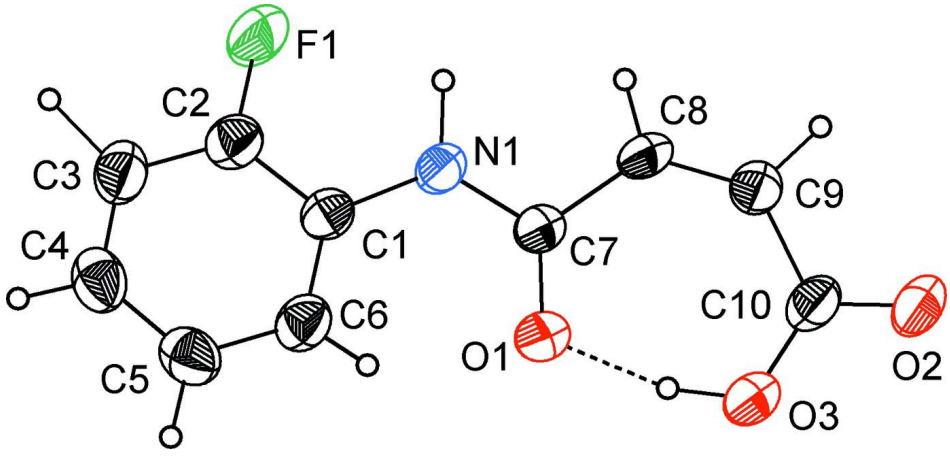


Figure 1

The molecular structure of the title compound. Thermal ellipsoids are drawn at the 50% probability level. The intramolecular O—H···O hydrogen bond is shown as a dashed line.

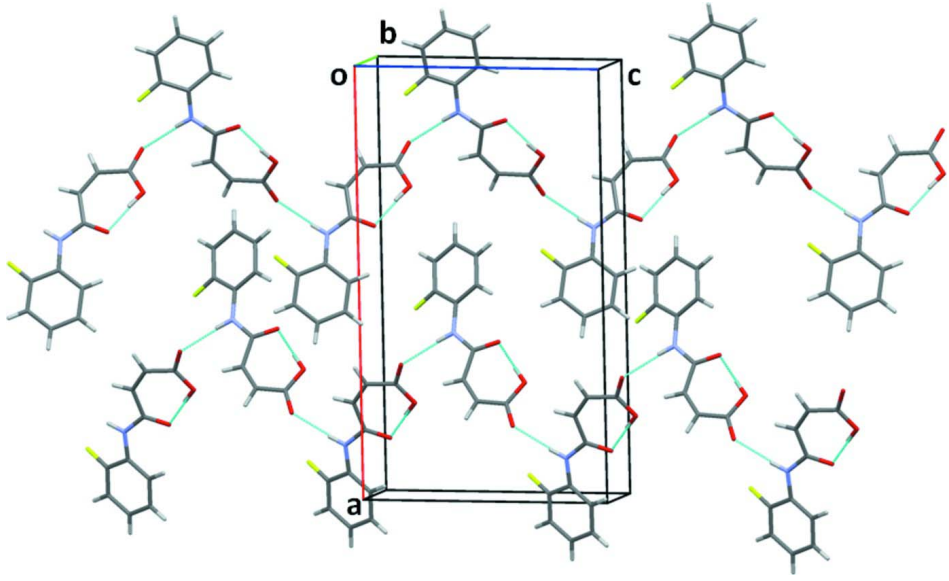


Figure 2

A view along the *b* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed cyan lines (see Table 1 for details).

(*Z*)-3-[(2-Fluoroanilino)carbonyl]prop-2-enoic acid

Crystal data

$C_{10}H_8FNO_3$
$M_r = 209.17$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 20.282\ (2)$ Å
$b = 3.8025\ (4)$ Å
$c = 11.8183\ (8)$ Å
$V = 911.45\ (15)$ Å^3
$Z = 4$
$F(000) = 432$
$D_x = 1.524$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 49 reflections
$\theta = 6.2$–$19.7°$
$\mu = 0.13$ mm^{-1}
$T = 299$ K
Plate, yellow
0.57 × 0.21 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
7575 measured reflections
1075 independent reflections
799 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 27.5°$, $\theta_{min} = 5.3°$
$h = -24 \rightarrow 26$
$k = -4 \rightarrow 4$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.121$
$S = 1.09$
1075 reflections
132 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.3218P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.06487 (13)	0.1290 (8)	0.1972 (2)	0.0682 (9)
O1	0.13208 (13)	0.4940 (9)	0.5666 (2)	0.0568 (9)
O2	0.31277 (15)	1.0159 (9)	0.6674 (3)	0.0608 (10)
O3	0.21896 (15)	0.7409 (10)	0.6947 (3)	0.0609 (12)
N1	0.11309 (15)	0.4479 (9)	0.3789 (3)	0.0380 (10)
C1	0.04662 (8)	0.3316 (7)	0.38017 (19)	0.0339 (10)
C2	0.02363 (10)	0.1799 (7)	0.28070 (18)	0.0440 (12)
C3	−0.04193 (11)	0.0770 (7)	0.2720 (2)	0.0510 (16)
C4	−0.08451 (9)	0.1257 (8)	0.3629 (2)	0.0500 (15)
C5	−0.06152 (10)	0.2773 (8)	0.4623 (2)	0.0491 (15)
C6	0.00405 (11)	0.3803 (7)	0.47100 (17)	0.0436 (11)
C7	0.15083 (18)	0.5352 (10)	0.4677 (3)	0.0376 (11)
C8	0.21585 (19)	0.6799 (11)	0.4379 (3)	0.0418 (11)
C9	0.26209 (19)	0.8086 (11)	0.5039 (3)	0.0426 (11)
C10	0.2656 (2)	0.8609 (12)	0.6285 (3)	0.0433 (14)
H1A	0.132 (2)	0.467 (11)	0.317 (4)	0.040 (12)*
H3	−0.05730	−0.02450	0.20550	0.0610*

H3B	0.190 (4)	0.630 (18)	0.647 (7)	0.11 (2)*
H4	−0.12840	0.05680	0.35710	0.0600*
H5	−0.09000	0.30990	0.52310	0.0590*
H6	0.01940	0.48170	0.53760	0.0520*
H8	0.22570	0.68040	0.36100	0.0500*
H9	0.29970	0.88070	0.46550	0.0510*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0578 (14)	0.107 (2)	0.0399 (13)	−0.0096 (15)	0.0025 (12)	−0.0258 (14)
O1	0.0460 (14)	0.096 (2)	0.0283 (14)	−0.0165 (15)	−0.0017 (13)	0.0017 (16)
O2	0.0468 (16)	0.093 (2)	0.0425 (17)	−0.0111 (16)	−0.0097 (14)	−0.0176 (17)
O3	0.0479 (16)	0.101 (3)	0.0337 (15)	−0.0106 (18)	−0.0026 (14)	−0.0121 (19)
N1	0.0357 (15)	0.050 (2)	0.0284 (16)	0.0003 (14)	−0.0007 (15)	−0.0046 (16)
C1	0.0368 (17)	0.0353 (18)	0.0297 (19)	0.0044 (15)	−0.0042 (16)	0.0032 (16)
C2	0.044 (2)	0.046 (2)	0.042 (2)	0.0008 (18)	−0.003 (2)	0.001 (2)
C3	0.052 (2)	0.049 (3)	0.052 (3)	−0.0084 (19)	−0.017 (2)	0.003 (2)
C4	0.0400 (19)	0.054 (3)	0.056 (3)	−0.0057 (18)	−0.007 (2)	0.017 (2)
C5	0.0363 (18)	0.062 (3)	0.049 (3)	0.0049 (18)	0.0005 (19)	0.015 (2)
C6	0.0417 (19)	0.049 (2)	0.040 (2)	0.0044 (18)	−0.0049 (18)	0.001 (2)
C7	0.0366 (19)	0.046 (2)	0.0302 (19)	0.0001 (16)	0.0000 (17)	−0.0015 (19)
C8	0.043 (2)	0.058 (2)	0.0244 (17)	−0.0028 (19)	0.0019 (16)	−0.0086 (17)
C9	0.0339 (18)	0.059 (2)	0.035 (2)	−0.0034 (18)	0.0026 (16)	−0.0062 (19)
C10	0.037 (2)	0.059 (3)	0.034 (2)	0.0081 (19)	−0.0041 (18)	−0.008 (2)

Geometric parameters (Å, º)

F1—C2	1.308 (3)	C4—C5	1.3892
O1—C7	1.239 (4)	C5—C6	1.3902
O2—C10	1.214 (5)	C7—C8	1.472 (5)
O3—C10	1.310 (5)	C8—C9	1.314 (5)
O3—H3B	0.92 (8)	C9—C10	1.488 (5)
N1—C1	1.419 (4)	C3—H3	0.9300
N1—C7	1.341 (5)	C4—H4	0.9300
N1—H1A	0.83 (5)	C5—H5	0.9300
C1—C6	1.3900	C6—H6	0.9300
C1—C2	1.3900	C8—H8	0.9300
C2—C3	1.3899	C9—H9	0.9300
C3—C4	1.3908		
C10—O3—H3B	105 (5)	C7—C8—C9	129.5 (3)
C1—N1—C7	127.7 (3)	C8—C9—C10	132.2 (4)
C1—N1—H1A	118 (3)	O2—C10—O3	120.8 (4)
C7—N1—H1A	114 (3)	O2—C10—C9	118.5 (4)
N1—C1—C2	116.1 (2)	O3—C10—C9	120.7 (4)
N1—C1—C6	123.8 (2)	C2—C3—H3	120.00
C2—C1—C6	120.00	C4—C3—H3	120.00

C1—C2—C3	120.02	C3—C4—H4	120.00
F1—C2—C1	119.0 (2)	C5—C4—H4	120.00
F1—C2—C3	121.0 (2)	C4—C5—H5	120.00
C2—C3—C4	119.96	C6—C5—H5	120.00
C3—C4—C5	120.00	C1—C6—H6	120.00
C4—C5—C6	120.04	C5—C6—H6	120.00
C1—C6—C5	119.97	C7—C8—H8	115.00
O1—C7—N1	122.1 (3)	C9—C8—H8	115.00
O1—C7—C8	123.2 (3)	C8—C9—H9	114.00
N1—C7—C8	114.6 (3)	C10—C9—H9	114.00
C7—N1—C1—C2	−165.3 (3)	F1—C2—C3—C4	178.4 (3)
C7—N1—C1—C6	18.5 (5)	C1—C2—C3—C4	−0.04
C1—N1—C7—O1	6.3 (6)	C2—C3—C4—C5	0.04
C1—N1—C7—C8	−174.2 (3)	C3—C4—C5—C6	−0.02
N1—C1—C2—F1	5.3 (4)	C4—C5—C6—C1	0.00
N1—C1—C2—C3	−176.3 (3)	O1—C7—C8—C9	−5.0 (7)
C6—C1—C2—F1	−178.4 (3)	N1—C7—C8—C9	175.4 (4)
C6—C1—C2—C3	0.03	C7—C8—C9—C10	−1.3 (8)
N1—C1—C6—C5	176.0 (3)	C8—C9—C10—O2	−173.7 (5)
C2—C1—C6—C5	−0.02	C8—C9—C10—O3	6.6 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*B*···O1	0.92 (8)	1.60 (8)	2.506 (4)	170 (7)
N1—H1*A*···O2^{i}	0.83 (5)	2.10 (5)	2.929 (5)	175 (4)

Symmetry code: (i) −*x*+1/2, *y*−1/2, *z*−1/2.