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## Structure Reports

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## 3-[4-(Trifluoromethyl)phenyl]propanoic acid

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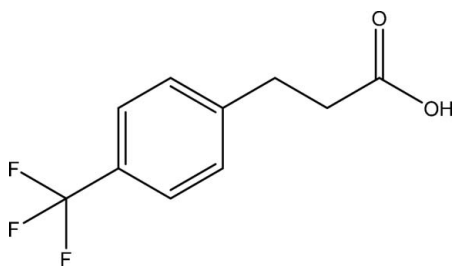
Received 16 March 2009; accepted 19 March 2009

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å; disorder in main residue;  $R$  factor = 0.068;  $wR$  factor = 0.178; data-to-parameter ratio = 13.7.

In crystal of the the title compound,  $\text{C}_{10}\text{H}_9\text{F}_3\text{O}_2$ , inversion dimers linked by pairs of  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds occur.

### Related literature

For bond-length data, see: Allen *et al.* (1987). For related literature on acid derivatives, see: Battistuzzi *et al.* (2003); Feuerstein *et al.* (2001, 2003); Johnson & Wen (1981); Shoda & Kuriyama (2003); Yamanouchi & Yamane (1988).



### Experimental

#### Crystal data

$\text{C}_{10}\text{H}_9\text{F}_3\text{O}_2$   
 $M_r = 218.17$   
Triclinic,  $P\bar{1}$   
 $a = 7.9028$  (19) Å  
 $b = 8.288$  (2) Å  
 $c = 9.238$  (3) Å

$\alpha = 63.381$  (15)°  
 $\beta = 85.20$  (3)°  
 $\gamma = 65.70$  (2)°  
 $V = 489.2$  (2) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation

$\mu = 0.14$  mm<sup>-1</sup>  
 $T = 298$  K

0.20 × 0.10 × 0.10 mm

#### Data collection

Enraf–Nonius CAD-4  
diffractometer  
Absorption correction:  $\psi$  scan  
(North *et al.*, 1968)  
 $T_{\min} = 0.973$ ,  $T_{\max} = 0.986$   
1894 measured reflections

1754 independent reflections  
874 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.017$   
3 standard reflections  
every 200 reflections  
intensity decay: 1%

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$   
 $wR(F^2) = 0.178$   
 $S = 1.00$   
1754 reflections

128 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.17$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1A}\cdots\text{O2}^i$	0.82	1.87	2.687 (4)	174

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2744).

### References

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**supplementary materials**

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### 3-[4-(Trifluoromethyl)phenyl]propanoic acid

J.-N. Guan, X.-J. Kong, B. Xu, J.-H. Liang and N. Song

#### Comment

Some derivatives of acids is important chemical material (Battistuzzi *et al.*, 2003; Feuerstein *et al.*, 2003, 2001; Johnson & Wen, 1981; Yamanouchi & Yamane 1988; Shoda & Kuriyama, 2003). We report here the crystal structure of the title compound, (I). The molecular structure of (I) is shown in Fig. 1, and the selected geometric parameters are given in Table 1. The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).

In the crystal of the title compound, there is an intermolecular O—H···O hydrogen bond which may be effective to the stabilization of the crystal.

#### Experimental

2,2-Dimethyl-5-(4-trifluoromethyl-benzyl)-[1,3]dioxane-4,6-dione (1 mmol), acetonitrile (25 ml) and water (0.25 ml) were mixed and subjected to microwave irradiation at 120° for 30 min (150 psi, 300 W, run time 5 min, hold time 30 min). Crude compound (I) was obtained. An X-ray grade crystal of (I) (500 mg) was grown from ethyl ether (10 ml) at room temperature.

#### Refinement

H atoms were placed geometrically at the distances of C—H = 0.93–0.97 Å and O—H = 0.82 Å, and included in the refinement in riding motion approximation with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5U_{\text{eq}}$  of the carrier atom.

#### Figures

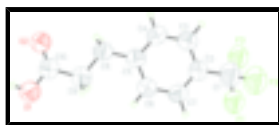


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids at the 30% probability level.

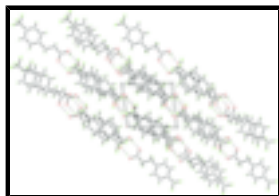


Fig. 2. View of the packing and hydrogen bonding interactions of (I).

### 3-[4-(Trifluoromethyl)phenyl]propanoic acid

#### Crystal data

$\text{C}_{10}\text{H}_9\text{F}_3\text{O}_2$   
 $M_r = 218.17$

$Z = 2$   
 $F_{000} = 224$

# supplementary materials

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Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 7.9028$  (19) Å

$b = 8.288$  (2) Å

$c = 9.238$  (3) Å

$\alpha = 63.381$  (15)°

$\beta = 85.20$  (3)°

$\gamma = 65.70$  (2)°

$V = 489.2$  (2) Å<sup>3</sup>

$D_x = 1.481$  Mg m<sup>-3</sup>

Melting point: 379 K

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 25 reflections

$\theta = 9\text{--}12^\circ$

$\mu = 0.14$  mm<sup>-1</sup>

$T = 298$  K

Yellow, colourless

0.20 × 0.10 × 0.10 mm

## Data collection

Enraf–Nonius CAD-4  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$  K

$\omega/2\theta$  scans

Absorption correction:  $\psi$  scan  
(North *et al.*, 1968)

$T_{\min} = 0.973$ ,  $T_{\max} = 0.986$

1894 measured reflections

1754 independent reflections

874 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\text{max}} = 25.3^\circ$

$\theta_{\text{min}} = 2.5^\circ$

$h = 0\text{--}9$

$k = -9\text{--}9$

$l = -11\text{--}11$

3 standard reflections

every 200 reflections

intensity decay: 1%

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.068$

$wR(F^2) = 0.178$

$S = 1.00$

1754 reflections

128 parameters

Primary atom site location: structure-invariant direct  
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring  
sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.216P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.19$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.17$  e Å<sup>-3</sup>

Extinction correction: none

## 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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.7456 (3)	-0.0616 (4)	1.0251 (3)	0.0961 (9)	
H1A	0.6554	-0.0765	1.0699	0.144*	
O2	0.5346 (4)	0.1263 (4)	0.8086 (3)	0.0888 (9)	
F1	1.5281 (8)	0.2427 (10)	0.2421 (7)	0.1096 (8)	0.429 (2)
F2	1.3838 (9)	0.5350 (11)	0.1735 (8)	0.1096 (8)	0.429 (2)
F3	1.3223 (9)	0.3992 (11)	0.0426 (8)	0.1096 (8)	0.429 (2)
F1'	1.4156 (7)	0.2852 (8)	0.1174 (6)	0.1096 (8)	0.571 (2)
F2'	1.4908 (7)	0.3848 (8)	0.2634 (6)	0.1096 (8)	0.571 (2)
F3'	1.2747 (6)	0.5871 (7)	0.0624 (6)	0.1096 (8)	0.571 (2)
C1	1.3412 (7)	0.3971 (8)	0.1896 (6)	0.1096 (8)	
C2	1.2089 (5)	0.3532 (5)	0.2963 (4)	0.0649 (9)	
C3	1.0233 (5)	0.4424 (6)	0.2356 (5)	0.0865 (12)	
H3A	0.9861	0.5349	0.1262	0.104*	
C4	0.8919 (5)	0.3987 (6)	0.3320 (5)	0.0906 (13)	
H4A	0.7682	0.4591	0.2857	0.109*	
C5	0.9377 (5)	0.2676 (5)	0.4958 (4)	0.0628 (9)	
C6	1.1224 (5)	0.1850 (7)	0.5566 (5)	0.0921 (13)	
H6A	1.1592	0.0968	0.6670	0.111*	
C7	1.2561 (5)	0.2288 (6)	0.4585 (4)	0.0827 (12)	
H7A	1.3794	0.1723	0.5046	0.099*	
C8	0.7910 (5)	0.2231 (6)	0.5981 (4)	0.0780 (11)	
H8A	0.7335	0.1714	0.5508	0.094*	
H8B	0.6948	0.3479	0.5891	0.094*	
C9	0.8489 (5)	0.0810 (5)	0.7754 (4)	0.0756 (11)	
H9A	0.9393	-0.0470	0.7859	0.091*	
H9B	0.9113	0.1283	0.8231	0.091*	
C10	0.6946 (6)	0.0527 (6)	0.8697 (5)	0.0716 (10)	

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0801 (18)	0.104 (2)	0.0801 (18)	-0.0392 (16)	0.0072 (14)	-0.0214 (16)
O2	0.0765 (18)	0.100 (2)	0.0808 (17)	-0.0409 (16)	0.0095 (14)	-0.0300 (15)
F1	0.1028 (18)	0.119 (2)	0.1119 (18)	-0.0560 (17)	0.0344 (13)	-0.0514 (15)
F2	0.1028 (18)	0.119 (2)	0.1119 (18)	-0.0560 (17)	0.0344 (13)	-0.0514 (15)
F3	0.1028 (18)	0.119 (2)	0.1119 (18)	-0.0560 (17)	0.0344 (13)	-0.0514 (15)
F1'	0.1028 (18)	0.119 (2)	0.1119 (18)	-0.0560 (17)	0.0344 (13)	-0.0514 (15)
F2'	0.1028 (18)	0.119 (2)	0.1119 (18)	-0.0560 (17)	0.0344 (13)	-0.0514 (15)
F3'	0.1028 (18)	0.119 (2)	0.1119 (18)	-0.0560 (17)	0.0344 (13)	-0.0514 (15)

## supplementary materials

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C1	0.1028 (18)	0.119 (2)	0.1119 (18)	-0.0560 (17)	0.0344 (13)	-0.0514 (15)
C2	0.075 (2)	0.060 (2)	0.073 (2)	-0.032 (2)	0.0156 (18)	-0.0384 (19)
C3	0.074 (3)	0.085 (3)	0.074 (2)	-0.025 (2)	0.004 (2)	-0.021 (2)
C4	0.064 (2)	0.095 (3)	0.088 (3)	-0.025 (2)	0.007 (2)	-0.029 (2)
C5	0.067 (2)	0.064 (2)	0.067 (2)	-0.0261 (18)	0.0045 (17)	-0.0388 (18)
C6	0.080 (3)	0.108 (3)	0.071 (2)	-0.042 (3)	0.003 (2)	-0.023 (2)
C7	0.073 (2)	0.108 (3)	0.073 (2)	-0.045 (2)	0.0032 (19)	-0.039 (2)
C8	0.069 (2)	0.102 (3)	0.070 (2)	-0.039 (2)	0.0010 (18)	-0.042 (2)
C9	0.079 (2)	0.067 (2)	0.082 (2)	-0.030 (2)	0.016 (2)	-0.037 (2)
C10	0.081 (3)	0.069 (3)	0.082 (3)	-0.040 (2)	0.016 (2)	-0.042 (2)

### *Geometric parameters (Å, °)*

O1—C10	1.298 (4)	C4—C5	1.377 (5)
O1—H1A	0.8200	C4—H4A	0.9300
O2—C10	1.211 (4)	C5—C6	1.373 (5)
F1—C1	1.436 (8)	C5—C8	1.493 (5)
F2—C1	1.264 (8)	C6—C7	1.389 (5)
F3—C1	1.371 (8)	C6—H6A	0.9300
F1'—C1	1.300 (6)	C7—H7A	0.9300
F2'—C1	1.359 (6)	C8—C9	1.494 (5)
F3'—C1	1.379 (6)	C8—H8A	0.9700
C1—C2	1.420 (5)	C8—H8B	0.9700
C2—C7	1.357 (4)	C9—C10	1.475 (5)
C2—C3	1.373 (5)	C9—H9A	0.9700
C3—C4	1.367 (5)	C9—H9B	0.9700
C3—H3A	0.9300		
C10—O1—H1A	109.5	C3—C4—C5	121.8 (4)
F2—C1—F1'	124.1 (5)	C3—C4—H4A	119.1
F2—C1—F2'	50.9 (4)	C5—C4—H4A	119.1
F1'—C1—F2'	104.0 (5)	C6—C5—C4	116.1 (4)
F2—C1—F3	111.3 (5)	C6—C5—C8	123.3 (3)
F1'—C1—F3	40.0 (3)	C4—C5—C8	120.6 (3)
F2'—C1—F3	128.7 (5)	C5—C6—C7	122.1 (4)
F2—C1—F3'	53.5 (4)	C5—C6—H6A	119.0
F1'—C1—F3'	103.4 (5)	C7—C6—H6A	119.0
F2'—C1—F3'	102.5 (5)	C2—C7—C6	120.7 (4)
F3—C1—F3'	68.0 (4)	C2—C7—H7A	119.6
F2—C1—C2	119.6 (5)	C6—C7—H7A	119.6
F1'—C1—C2	116.3 (5)	C5—C8—C9	118.1 (3)
F2'—C1—C2	113.8 (4)	C5—C8—H8A	107.8
F3—C1—C2	115.5 (5)	C9—C8—H8A	107.8
F3'—C1—C2	115.2 (4)	C5—C8—H8B	107.8
F2—C1—F1	96.1 (5)	C9—C8—H8B	107.8
F1'—C1—F1	58.3 (4)	H8A—C8—H8B	107.1
F2'—C1—F1	50.5 (3)	C10—C9—C8	114.8 (3)
F3—C1—F1	95.9 (5)	C10—C9—H9A	108.6
F3'—C1—F1	130.2 (4)	C8—C9—H9A	108.6
C2—C1—F1	114.2 (4)	C10—C9—H9B	108.6

C7—C2—C3	117.5 (3)	C8—C9—H9B	108.6
C7—C2—C1	123.0 (4)	H9A—C9—H9B	107.5
C3—C2—C1	119.5 (4)	O2—C10—O1	122.4 (3)
C4—C3—C2	121.6 (4)	O2—C10—C9	123.5 (4)
C4—C3—H3A	119.2	O1—C10—C9	114.0 (4)
C2—C3—H3A	119.2		
F2—C1—C2—C7	-85.8 (7)	C2—C3—C4—C5	2.0 (7)
F1'—C1—C2—C7	92.3 (6)	C3—C4—C5—C6	0.5 (6)
F2'—C1—C2—C7	-28.5 (7)	C3—C4—C5—C8	179.9 (4)
F3—C1—C2—C7	137.0 (5)	C4—C5—C6—C7	-0.7 (6)
F3'—C1—C2—C7	-146.5 (5)	C8—C5—C6—C7	179.9 (4)
F1—C1—C2—C7	27.1 (7)	C3—C2—C7—C6	3.8 (6)
F2—C1—C2—C3	92.8 (7)	C1—C2—C7—C6	-177.6 (4)
F1'—C1—C2—C3	-89.2 (6)	C5—C6—C7—C2	-1.5 (7)
F2'—C1—C2—C3	150.0 (5)	C6—C5—C8—C9	-0.1 (5)
F3—C1—C2—C3	-44.4 (7)	C4—C5—C8—C9	-179.5 (4)
F3'—C1—C2—C3	32.0 (7)	C5—C8—C9—C10	177.0 (3)
F1—C1—C2—C3	-154.3 (5)	C8—C9—C10—O2	5.0 (5)
C7—C2—C3—C4	-4.1 (6)	C8—C9—C10—O1	-176.0 (3)
C1—C2—C3—C4	177.2 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1A...O2 <sup>i</sup>	0.82	1.87	2.687 (4)	174

Symmetry codes: (i)  $-x+1, -y, -z+2$ .

Fig. 1

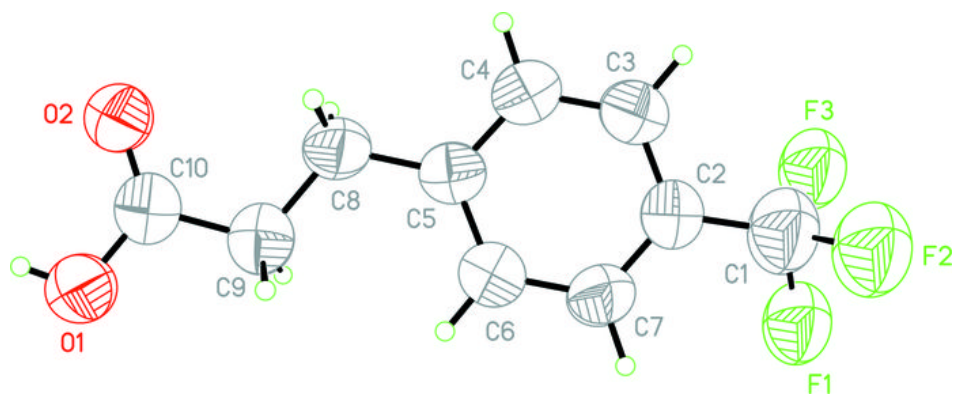




Fig. 2

