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

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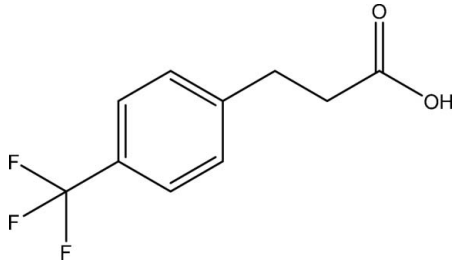
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.068; wR factor = 0.178; data-to-parameter ratio = 13.7.

In crystal of the the title compound, $C_{10}H_9F_3O_2$, inversion dimers linked by pairs of O—H···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

$C_{10}H_9F_3O_2$
M_r = 218.17
Triclinic, $P\overline{1}$
a = 7.9028 (19) Å
b = 8.288 (2) Å
c = 9.238 (3) Å
α = 63.381 (15)°
β = 85.20 (3)°
γ = 65.70 (2)°
V = 489.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 298 K
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ 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_{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^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···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

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Battistuzzi, G., Cacchi, S., Fabrizi, G. & Bernini, R. (2003). *Synlett*, pp. 1133–1136.
Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Feuerstein, M., Berthiol, F., Doucet, H. & Santelli, M. (2003). *Org. Biomol. Chem.* pp. 2235–2237.
Feuerstein, M., Laurenti, D., Bougeant, C., Doucet, H. & Santelli, M. (2001). *Chem. Commun.* pp. 325–326.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Johnson, P. Y. & Wen, J. Q. (1981). *J. Org. Chem.* **46**, 2767–2771.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shoda, K. & Kuriyama, H. (2003). PCT Int. Appl. WO, 2003 070 686.
Yamanouchi, T. & Yamane, H. (1988). Jpn Patent JP 63 250 356.

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

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S1. 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.

S2. 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.

S3. 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_{iso}(H) = 1.2 or 1.5U_{eq} of the carrier atom.

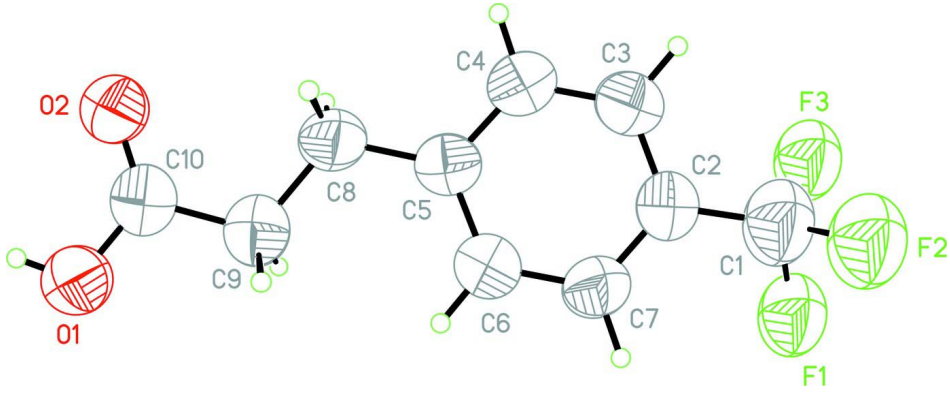

Figure 1

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

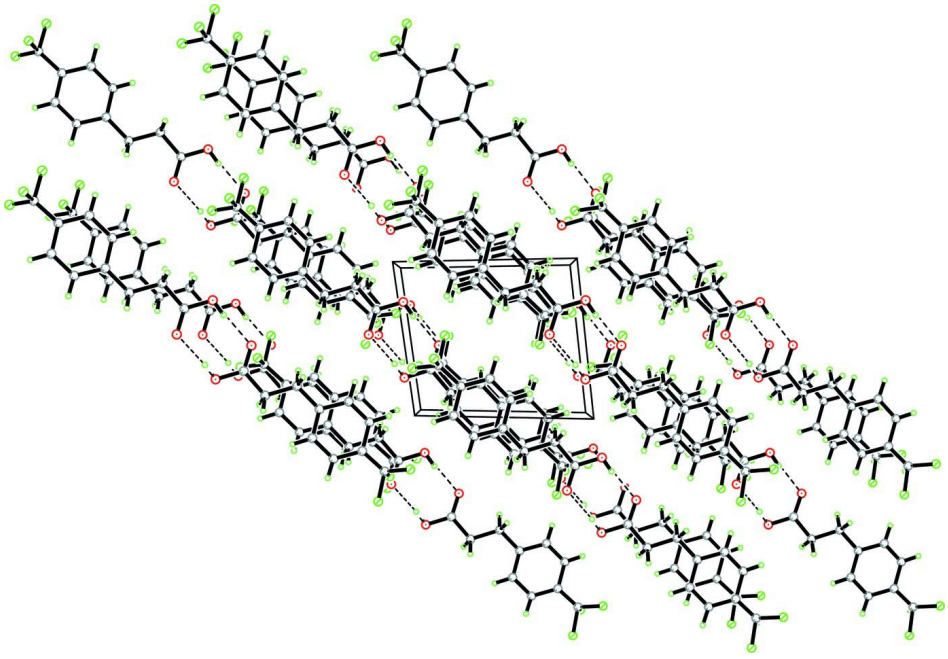

Figure 2

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

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Crystal data

$C_{10}H_9F_3O_2$
$M_r = 218.17$
Triclinic, $P\overline{1}$
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^3
$Z = 2$
$F(000) = 224$
$D_x = 1.481$ Mg m^{-3}
Melting point: 379 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–12°$
$\mu = 0.14$ mm^{-1}
$T = 298$ K
Yellow, colourless
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.973$, $T_{max} = 0.986$
1894 measured reflections
1754 independent reflections
874 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.5°$
$h = 0\rightarrow9$
$k = -9\rightarrow9$
$l = -11\rightarrow11$
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
0 restraints
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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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)
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, º)

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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2^{i}	0.82	1.87	2.687 (4)	174

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