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Diethyl pyrazine-2,5-dicarboxylate

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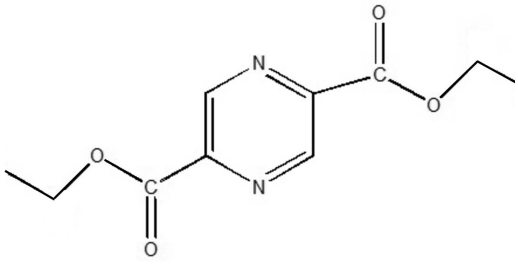
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.053; wR factor = 0.131; data-to-parameter ratio = 18.0.

The molecule of the title compound, $C_{10}H_{12}N_2O_4$, is located around an inversion center. The carboxylate groups are twisted slightly with respect to the pyrazine ring, making a dihedral angle of 2.76 (19)°. In the crystal, molecules are stacked along the c axis *via* weak C—H···O hydrogen bonds.

Related literature

For the structures of related compounds, see: Zhang *et al.* (2010); Cockriel *et al.* (2008).



Experimental

Crystal data

$C_{10}H_{12}N_2O_4$
M_r = 224.22
Monoclinic, $P2_1/c$
a = 12.284 (6) Å
b = 5.640 (3) Å
c = 7.881 (4) Å
β = 108.713 (9)°
V = 517.2 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 173 K
0.7 × 0.3 × 0.05 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.994
2994 measured reflections
1317 independent reflections
1055 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.131
S = 1.07
1317 reflections
73 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O2^{i}	0.97	2.58	3.537 (3)	168

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5143).

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supplementary materials

Acta Cryst. (2012). E**68**, o2236 [doi:10.1107/S1600536812028164]

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Comment

The structure of the title compound is illustrated in Fig. 1. The molecule of title compound, $C_{10}H_{12}N_2O_4$, is essentially planar and the carboxylate groups are twisted slightly with respect to the pyrazine ring, making a dihedral angle of 2.76 (19)°. The carboxyl C—O and C═O bonds are normal, while the bond angle of C—N═C are slightly larger than those in diisopropyl pyrazine-2,5-dicarboxylate (Zhang *et al.*, 2010). The angle C3—O1—C4 of 116.05° is larger compared to the value of 115.05° in pyrazine-2,5-dicarboxylic acid dimethyl ester (Cockriel *et al.*, 2008). The crystal structure is stabilized *via* van der Waals forces and week C—H···O hydrogen bonds (Fig. 2 and Table 1).

Experimental

The title compound was synthesized by dissolving 2,5-pyrazinedicarboxylic acid (2 g, 11.9 mmol) in 200 ml ethanol, while stirring 2 ml concentrated H_2SO_4 was added slowly. The solution was left to reflux for 12 h, then distillation under reduced pressure until no solution to outflow. The solution was made neutral with Na_2CO_3(aq), extracted with 30 ml ethyl acetate. Transparent crystals of the title compound were obtained by slow evaporation at room temperature for ten days.

Refinement

H atoms were included in a riding model approximation with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{mehtyl}) .

Computing details

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

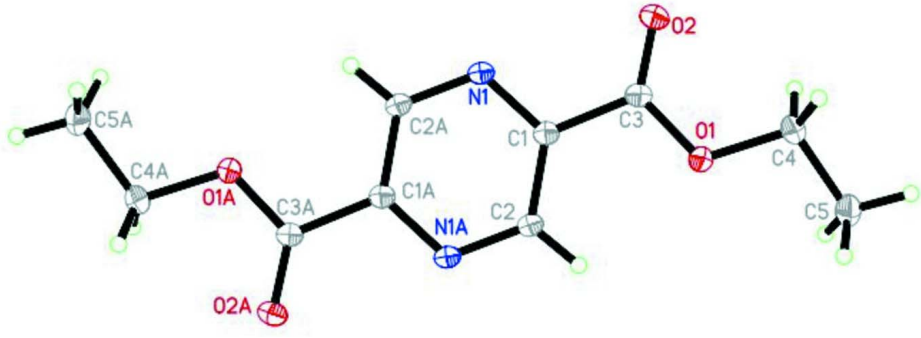

Figure 1

The molecular structure (at 30% probability) of the title compound. [Symmetry code: (A) 1 - *x*, -*y*, 1 - *z*].

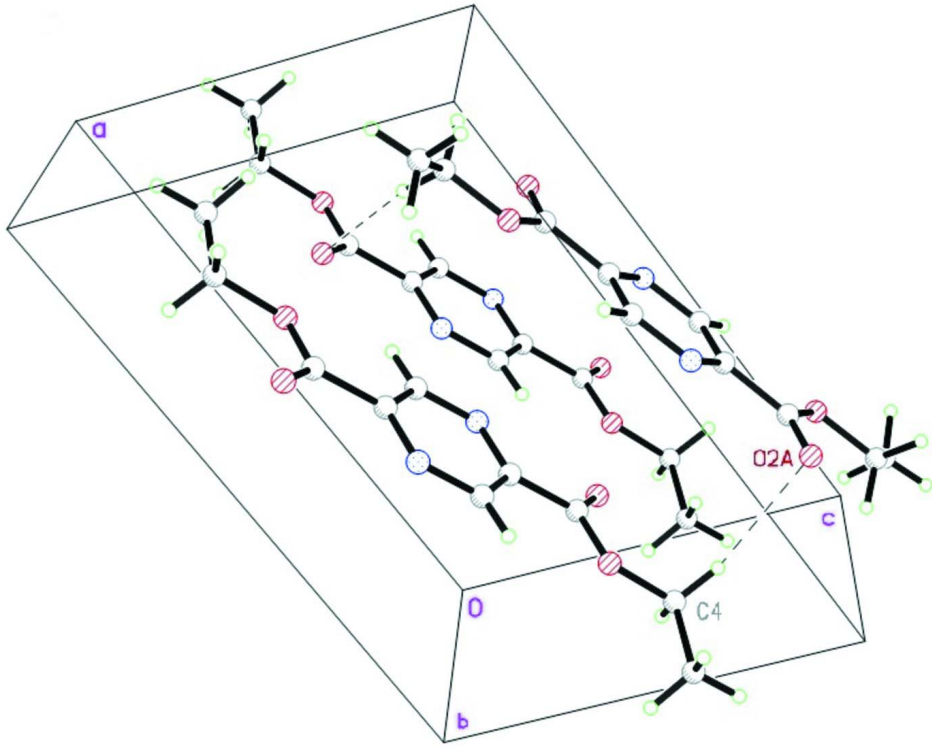

Figure 2

Packing diagram of the title complex, showing hydrogen bonds as dashed lines. [Symmetry code: (A) *x*, -0.5 - *y*, 0.5 + *z*].

Diethyl pyrazine-2,5-dicarboxylate

Crystal data

$C_{10}H_{12}N_2O_4$
$M_r = 224.22$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.284$ (6) Å
$b = 5.640$ (3) Å
$c = 7.881$ (4) Å
$\beta = 108.713$ (9)°
$V = 517.2$ (5) Å^3
$Z = 2$
$F(000) = 236.0$
$D_x = 1.440$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2994 reflections
$\theta = 4.0$–$28.5°$
$\mu = 0.11$ mm^{-1}
$T = 173$ K
Plate, colourless
0.7 × 0.3 × 0.05 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick,1996)
$T_{min} = 0.960$, $T_{max} = 0.994$
2994 measured reflections
1317 independent reflections
1055 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.5°$, $\theta_{min} = 4.0°$
$h = -16 \rightarrow 14$
$k = -5 \rightarrow 7$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.131$
$S = 1.07$
1317 reflections
73 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
$w = 1/[\sigma^2(F_o^2) + (0.0606P)^2 + 0.1472P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ 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}
N1	0.46961 (11)	−0.2315 (2)	0.52651 (18)	0.0275 (3)
O1	0.26007 (9)	0.0921 (2)	0.64425 (16)	0.0308 (3)
O2	0.28072 (11)	−0.3005 (2)	0.63126 (19)	0.0401 (4)
C1	0.41208 (12)	−0.0450 (3)	0.55512 (19)	0.0241 (3)
C2	0.44174 (13)	0.1860 (3)	0.5289 (2)	0.0265 (4)
H2A	0.3986	0.3110	0.5507	0.032*
C3	0.31162 (13)	−0.1030 (3)	0.6147 (2)	0.0265 (4)
C4	0.16106 (15)	0.0568 (3)	0.7018 (3)	0.0359 (4)
H4A	0.1848	0.0010	0.8247	0.043*
H4B	0.1102	−0.0605	0.6266	0.043*
C5	0.10095 (15)	0.2883 (3)	0.6871 (2)	0.0377 (4)
H5A	0.0725	0.3356	0.5636	0.057*
H5B	0.1537	0.4058	0.7549	0.057*
H5C	0.0378	0.2732	0.7333	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0314 (7)	0.0174 (6)	0.0369 (7)	−0.0001 (5)	0.0154 (6)	0.0002 (5)
O1	0.0289 (6)	0.0234 (6)	0.0457 (7)	0.0012 (4)	0.0199 (5)	0.0006 (5)
O2	0.0450 (8)	0.0234 (7)	0.0617 (9)	−0.0062 (5)	0.0307 (6)	−0.0005 (6)
C1	0.0256 (7)	0.0211 (8)	0.0256 (7)	−0.0009 (6)	0.0080 (6)	−0.0005 (6)
C2	0.0304 (8)	0.0184 (7)	0.0328 (8)	0.0014 (6)	0.0132 (6)	0.0000 (6)
C3	0.0284 (8)	0.0212 (8)	0.0304 (8)	−0.0010 (6)	0.0104 (6)	0.0007 (6)
C4	0.0330 (9)	0.0337 (9)	0.0493 (10)	0.0000 (7)	0.0247 (8)	0.0048 (8)
C5	0.0330 (9)	0.0410 (11)	0.0450 (10)	0.0046 (7)	0.0208 (8)	0.0018 (8)

Geometric parameters (Å, º)

N1—C2^{i}	1.322 (2)	C2—H2A	0.9300
N1—C1	1.326 (2)	C4—C5	1.486 (3)
O1—C3	1.3270 (19)	C4—H4A	0.9700
O1—C4	1.442 (2)	C4—H4B	0.9700
O2—C3	1.197 (2)	C5—H5A	0.9600
C1—C2	1.386 (2)	C5—H5B	0.9600
C1—C3	1.490 (2)	C5—H5C	0.9600
C2^{i}—N1—C1	116.31 (14)	O1—C4—H4A	110.2
C3—O1—C4	116.04 (13)	C5—C4—H4A	110.2
N1—C1—C2	122.69 (14)	O1—C4—H4B	110.2
N1—C1—C3	114.83 (14)	C5—C4—H4B	110.2
C2—C1—C3	122.47 (14)	H4A—C4—H4B	108.5
N1^{i}—C2—C1	121.00 (15)	C4—C5—H5A	109.5
N1^{i}—C2—H2A	119.5	C4—C5—H5B	109.5
C1—C2—H2A	119.5	H5A—C5—H5B	109.5
O2—C3—O1	124.49 (15)	C4—C5—H5C	109.5
O2—C3—C1	124.19 (15)	H5A—C5—H5C	109.5
O1—C3—C1	111.31 (13)	H5B—C5—H5C	109.5
O1—C4—C5	107.59 (14)		
C2^{i}—N1—C1—C2	0.1 (3)	N1—C1—C3—O2	−2.3 (2)
C2^{i}—N1—C1—C3	179.07 (13)	C2—C1—C3—O2	176.70 (16)
N1—C1—C2—N1^{i}	−0.1 (3)	N1—C1—C3—O1	178.63 (13)
C3—C1—C2—N1^{i}	−178.99 (14)	C2—C1—C3—O1	−2.4 (2)
C4—O1—C3—O2	0.6 (2)	C3—O1—C4—C5	−167.24 (14)
C4—O1—C3—C1	179.71 (13)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O2^{ii}	0.97	2.58	3.537 (3)	168

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