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N-(3,4-Diethoxyphenyl)acetamide

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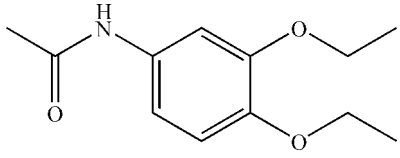
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.119; data-to-parameter ratio = 14.9.

In the title compound, $C_{12}H_{17}NO_3$, the conformations of the N—H and C═O bonds are *anti* to each other. In the crystal structure, N—H···O hydrogen-bond interactions help to establish the packing.

Related literature

For the use of acetamides in the synthesis of biologically active compounds, see: Koike *et al.* (1999). The benzanilide core is present in compounds with a wide range of biological activity and benzanilides and benzamides are also used extensively in organic synthesis (Saeed *et al.*, 2008). Various *N*-substituted benzamides exhibit potent antiemetic activity, see: Vega-Noverola *et al.* (1989).



Experimental

Crystal data

$C_{12}H_{17}NO_3$
M_r = 223.27
Monoclinic, $P2_1/c$
a = 15.563 (8) Å
b = 8.661 (6) Å
c = 9.305 (7) Å
β = 101.773 (14)°
V = 1227.8 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.24 × 0.21 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.971, T_{max} = 0.975
6295 measured reflections
2155 independent reflections
1570 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.119
S = 1.08
2155 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.86	2.08	2.915 (2)	164

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2786).

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supplementary materials

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N-(3,4-Diethoxyphenyl)acetamide

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Comment

Acetamide is an important class of medical intermidate. Many biologically active compounds are synthesized by using acetamide (Koike *et al.*, 1999). The benzanilide core is present in compounds with a wide range of biological activity and benzanilides and benzamides are also used extensively in organic synthesis (Saeed *et al.*, 2008). Various N-substituted benzamides exhibit potent antiemetic activity (Vega-Noverola *et al.*, 1989). The crystal structure determination of the title compound (I) has been carried out in order to elucidate the molecular conformation.

The molecule of the title compound, (Fig. 1), consists of a phenylacetamide group and two ethoxyl groups. The conformations of the N—H and C=O bonds are anti to each other. The C10—C9—O2—C4 and C8—C7—O1—C3 torsion angles are -173.61 (15)° and 178.46 (15)°, respectively. The title compound forms intermolecular H bonds whereas the N1 act as hydrogen-bond donor and the O3 act as hydrogen-bond acceptor, the distance of the N1—H1···O3 hydrogen bond is 2.915 (2) Å (Table 1). In the crystal structure, N—H···O hydrogen bonds interactions may help to establish the packing.

Experimental

Ferrous powder (2.20 g, 0.039 mol), water (15 ml) and acetic acid (3 ml) were reflux for 4 h, the reaction mixture was cooled to room temperature. Then a solution of 1,2-diethoxy-4-nitrobenzene (2.10 g, 0.01 mol) in acetic acid (50 ml) was added to the mixture, the solution was reflux for 6 h. the mixture was filtered, and the resulting solution was added to water (150 ml), much white precipitate was appeared, the mixture was filtered again, the solid product was dissolved in 80 ml ethanol. and then set aside for five days to obtain colourless crystals [yield: 53%].

Refinement

All other H atoms were placed in calculated positions and refined as riding, with C—H = 0.93–0.97 Å, N—H = 0.86 Å, and U_{iso}(H) = 1.2–1.5 U_{eq}(C,*N*).

Figures

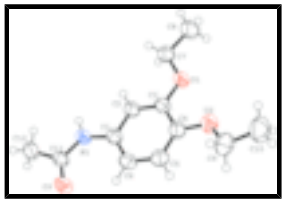

Fig. 1. The molecular structure of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

N-(3,4-Diethoxyphenyl)acetamide

Crystal data

$C_{12}H_{17}NO_3$	$F_{000} = 480$
$M_r = 223.27$	$D_x = 1.208$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2155 reflections
$a = 15.563$ (8) Å	$\theta = 1.3$–25.0º
$b = 8.661$ (6) Å	$\mu = 0.09$ mm^{-1}
$c = 9.305$ (7) Å	$T = 293$ K
$\beta = 101.773$ (14)º	Block, colourless
$V = 1227.8$ (14) Å^3	0.24 × 0.21 × 0.20 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2155 independent reflections
Radiation source: fine-focus sealed tube	1570 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
$T = 293$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.3$º
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -18\rightarrow16$
$T_{min} = 0.971$, $T_{max} = 0.975$	$k = -10\rightarrow10$
6295 measured reflections	$l = -10\rightarrow11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
2155 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
145 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.36147 (10)	0.08455 (17)	0.48242 (16)	0.0426 (4)
C2	0.32424 (10)	0.07894 (18)	0.60656 (15)	0.0451 (4)
H2	0.3519	0.1289	0.6920	0.054*
C3	0.24680 (10)	0.00019 (18)	0.60451 (16)	0.0445 (4)
C4	0.20432 (11)	−0.07482 (19)	0.47506 (17)	0.0479 (4)
C5	0.24235 (11)	−0.0712 (2)	0.35439 (18)	0.0542 (5)
H5	0.2153	−0.1223	0.2693	0.065*
C6	0.32090 (11)	0.00790 (19)	0.35673 (17)	0.0513 (4)
H6	0.3458	0.0089	0.2739	0.062*
C7	0.24108 (11)	0.0806 (2)	0.84850 (17)	0.0554 (5)
H7A	0.2403	0.1891	0.8225	0.067*
H7B	0.3013	0.0508	0.8887	0.067*
C8	0.18566 (14)	0.0537 (3)	0.9582 (2)	0.0759 (6)
H8A	0.2081	0.1128	1.0451	0.114*
H8B	0.1866	−0.0541	0.9827	0.114*
H8C	0.1265	0.0850	0.9179	0.114*
C9	0.06962 (12)	−0.1888 (2)	0.3449 (2)	0.0656 (5)
H9A	0.0967	−0.2673	0.2944	0.079*
H9B	0.0573	−0.0991	0.2817	0.079*
C10	−0.01353 (12)	−0.2493 (3)	0.3827 (3)	0.0869 (7)
H10A	−0.0539	−0.2776	0.2942	0.130*
H10B	−0.0394	−0.1707	0.4330	0.130*
H10C	−0.0004	−0.3382	0.4449	0.130*
C11	0.48850 (10)	0.20423 (18)	0.39666 (17)	0.0446 (4)
C12	0.56454 (11)	0.3114 (2)	0.44698 (19)	0.0569 (5)
H12A	0.5671	0.3393	0.5476	0.085*
H12B	0.5570	0.4026	0.3872	0.085*
H12C	0.6181	0.2606	0.4383	0.085*
N1	0.43955 (8)	0.17335 (14)	0.49706 (14)	0.0459 (4)
H1	0.4583	0.2131	0.5824	0.055*
O1	0.20629 (7)	−0.01068 (13)	0.72098 (11)	0.0559 (4)
O2	0.12688 (7)	−0.14790 (14)	0.48136 (13)	0.0626 (4)
O3	0.47167 (8)	0.15207 (13)	0.27060 (12)	0.0587 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0448 (9)	0.0439 (9)	0.0407 (8)	0.0034 (7)	0.0126 (7)	0.0045 (7)
C2	0.0490 (10)	0.0488 (9)	0.0385 (9)	−0.0023 (7)	0.0114 (7)	−0.0007 (7)
C3	0.0481 (10)	0.0458 (9)	0.0427 (9)	−0.0007 (7)	0.0162 (7)	0.0006 (7)
C4	0.0476 (10)	0.0486 (10)	0.0475 (9)	−0.0042 (8)	0.0103 (7)	−0.0004 (7)
C5	0.0615 (11)	0.0593 (11)	0.0419 (9)	−0.0073 (9)	0.0105 (8)	−0.0074 (8)
C6	0.0602 (11)	0.0569 (10)	0.0398 (9)	−0.0008 (8)	0.0174 (8)	−0.0008 (8)
C7	0.0614 (11)	0.0640 (11)	0.0437 (9)	−0.0105 (9)	0.0172 (8)	−0.0088 (8)
C8	0.0879 (15)	0.0933 (15)	0.0524 (11)	−0.0225 (12)	0.0279 (10)	−0.0150 (10)
C9	0.0592 (12)	0.0656 (12)	0.0658 (12)	−0.0083 (9)	−0.0018 (9)	−0.0002 (9)
C10	0.0583 (13)	0.0939 (17)	0.1049 (17)	−0.0174 (12)	0.0083 (12)	−0.0065 (13)
C11	0.0517 (10)	0.0432 (9)	0.0422 (9)	0.0096 (7)	0.0169 (7)	0.0094 (7)
C12	0.0590 (11)	0.0557 (10)	0.0611 (11)	−0.0030 (8)	0.0239 (9)	0.0089 (8)
N1	0.0501 (8)	0.0527 (8)	0.0375 (7)	−0.0036 (6)	0.0151 (6)	0.0004 (6)
O1	0.0606 (8)	0.0681 (8)	0.0443 (6)	−0.0172 (6)	0.0226 (6)	−0.0093 (6)
O2	0.0585 (8)	0.0752 (9)	0.0550 (7)	−0.0218 (6)	0.0133 (6)	−0.0094 (6)
O3	0.0723 (8)	0.0664 (8)	0.0423 (7)	0.0002 (6)	0.0231 (6)	0.0029 (5)

Geometric parameters (Å, °)

C1—C6	1.380 (2)	C8—H8B	0.9600
C1—C2	1.395 (2)	C8—H8C	0.9600
C1—N1	1.421 (2)	C9—O2	1.439 (2)
C2—C3	1.382 (2)	C9—C10	1.503 (3)
C2—H2	0.9300	C9—H9A	0.9700
C3—O1	1.3636 (19)	C9—H9B	0.9700
C3—C4	1.409 (2)	C10—H10A	0.9600
C4—C5	1.372 (2)	C10—H10B	0.9600
C4—O2	1.3732 (19)	C10—H10C	0.9600
C5—C6	1.398 (2)	C11—O3	1.2342 (19)
C5—H5	0.9300	C11—N1	1.3471 (19)
C6—H6	0.9300	C11—C12	1.502 (2)
C7—O1	1.437 (2)	C12—H12A	0.9600
C7—C8	1.483 (2)	C12—H12B	0.9600
C7—H7A	0.9700	C12—H12C	0.9600
C7—H7B	0.9700	N1—H1	0.8600
C8—H8A	0.9600		
C6—C1—C2	119.30 (15)	H8A—C8—H8C	109.5
C6—C1—N1	125.16 (14)	H8B—C8—H8C	109.5
C2—C1—N1	115.54 (13)	O2—C9—C10	106.70 (16)
C3—C2—C1	120.95 (14)	O2—C9—H9A	110.4
C3—C2—H2	119.5	C10—C9—H9A	110.4
C1—C2—H2	119.5	O2—C9—H9B	110.4
O1—C3—C2	124.51 (14)	C10—C9—H9B	110.4
O1—C3—C4	115.80 (14)	H9A—C9—H9B	108.6

C2—C3—C4	119.69 (14)	C9—C10—H10A	109.5
C5—C4—O2	125.06 (15)	C9—C10—H10B	109.5
C5—C4—C3	118.91 (15)	H10A—C10—H10B	109.5
O2—C4—C3	116.03 (14)	C9—C10—H10C	109.5
C4—C5—C6	121.37 (15)	H10A—C10—H10C	109.5
C4—C5—H5	119.3	H10B—C10—H10C	109.5
C6—C5—H5	119.3	O3—C11—N1	123.10 (16)
C1—C6—C5	119.75 (15)	O3—C11—C12	121.56 (15)
C1—C6—H6	120.1	N1—C11—C12	115.32 (14)
C5—C6—H6	120.1	C11—C12—H12A	109.5
O1—C7—C8	107.94 (14)	C11—C12—H12B	109.5
O1—C7—H7A	110.1	H12A—C12—H12B	109.5
C8—C7—H7A	110.1	C11—C12—H12C	109.5
O1—C7—H7B	110.1	H12A—C12—H12C	109.5
C8—C7—H7B	110.1	H12B—C12—H12C	109.5
H7A—C7—H7B	108.4	C11—N1—C1	129.38 (14)
C7—C8—H8A	109.5	C11—N1—H1	115.3
C7—C8—H8B	109.5	C1—N1—H1	115.3
H8A—C8—H8B	109.5	C3—O1—C7	117.45 (13)
C7—C8—H8C	109.5	C4—O2—C9	117.83 (13)
C6—C1—C2—C3	−1.1 (2)	C4—C5—C6—C1	−0.2 (3)
N1—C1—C2—C3	178.02 (13)	O3—C11—N1—C1	−2.1 (2)
C1—C2—C3—O1	−179.99 (14)	C12—C11—N1—C1	176.25 (14)
C1—C2—C3—C4	−0.4 (2)	C6—C1—N1—C11	1.4 (2)
O1—C3—C4—C5	−178.74 (14)	C2—C1—N1—C11	−177.71 (14)
C2—C3—C4—C5	1.7 (2)	C2—C3—O1—C7	7.5 (2)
O1—C3—C4—O2	0.8 (2)	C4—C3—O1—C7	−172.04 (14)
C2—C3—C4—O2	−178.79 (14)	C8—C7—O1—C3	178.46 (15)
O2—C4—C5—C6	179.12 (15)	C5—C4—O2—C9	−17.2 (2)
C3—C4—C5—C6	−1.4 (3)	C3—C4—O2—C9	163.33 (15)
C2—C1—C6—C5	1.4 (2)	C10—C9—O2—C4	−173.61 (15)
N1—C1—C6—C5	−177.64 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.86	2.08	2.915 (2)	164

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

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