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N,*N*′-Bis(2-ethoxyphenyl)oxamide

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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 = 0.116
Data-to-parameter ratio = 15.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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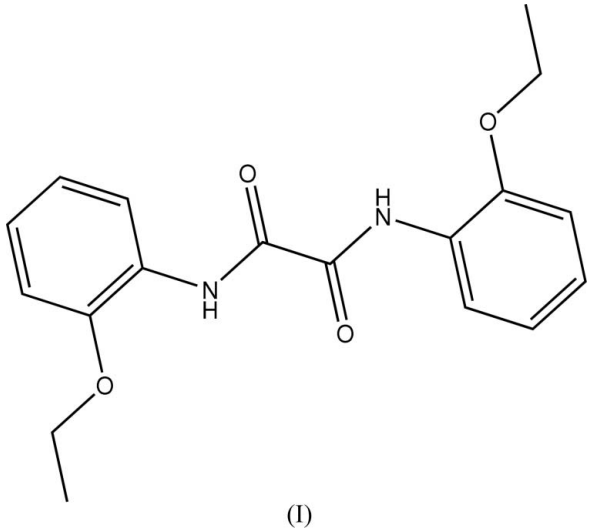
The title compound, $C_{18}H_{20}N_2O_4$, has an inversion center at the mid-point of the C—C bond of the oxamide unit. Intramolecular N—H···O and C—H···O hydrogen bonds make the molecule essentially planar.

Comment

We have recently reported the synthesis and crystal structure of *N*,*N*′-diphenyloxamide, (II) (Wen *et al.*, 2006). In our ongoing studies of oxamide derivatives, the title compound, (I), was obtained.



(I)

The compound (I) has an inversion center at the mid-point of the C—C bond of the oxamide unit (Fig. 1). The bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable to those in (II). The molecule of (I) is essentially planar, with the two ethoxy groups twisted slightly to opposite sides of the molecular plane [the dihedral angle between the main molecular plane and the OCC chain is 4.15 (2)°]. Intramolecular hydrogen bonds (Table 1) form five- and six-membered rings, contributing to the planarity of the molecule.

Experimental

To a solution of 2-ethoxyaniline (27.4 g, 0.2 mol) in benzene (90 ml) was added dropwise a solution of oxalyl chloride (6.4 g, 0.05 mol) in benzene (30 ml), and the mixture was stirred at 343 K for 8 h. After cooling to room temperature, water (50 ml) was added to the reaction mixture and the organic phase was washed three times with water to obtain (I) as a solid (yield 62%). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an *N*,*N*-dimethylformamide solution over a period of 9 h.

Crystal data

$C_{18}H_{20}N_2O_4$
M_r = 328.36
Monoclinic, $P2_1/c$
a = 8.7343 (10) Å
b = 14.5983 (16) Å
c = 7.1682 (8) Å
β = 110.157 (2)°
V = 858.01 (17) Å^3
Z = 2
D_x = 1.271 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Column, colorless
0.32 × 0.16 × 0.12 mm

Data collection

Siemens SMART 1000 CCD area detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.989
4858 measured reflections
1675 independent reflections
1208 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
S = 1.05
1675 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.0318P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	2.15	2.576 (2)	110
N1—H1A···O2^{i}	0.86	2.23	2.668 (2)	112
C7—H7A···O2	0.93	2.39	2.976 (2)	121

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N) and 1.5U_{eq}(methyl C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

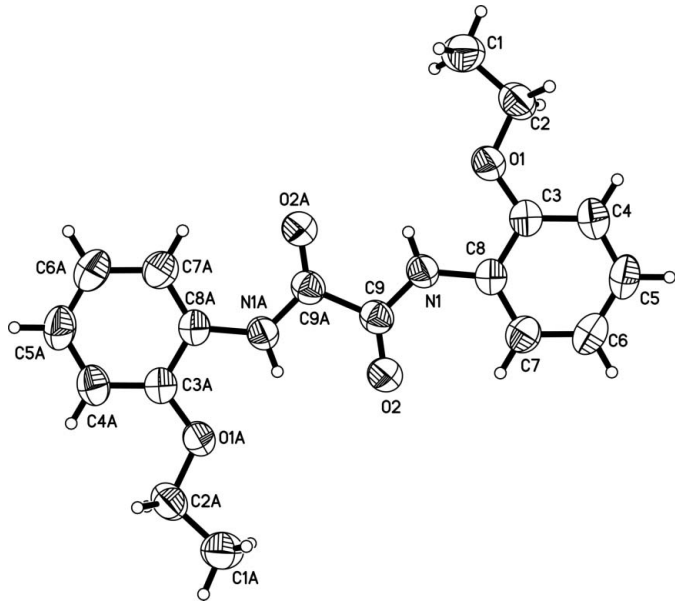


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The suffix A corresponds to symmetry code $(1-x, 1-y, 1-z)$.

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