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N,*N*′-Diphenylsuccinamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.114
Data-to-parameter ratio = 14.3

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

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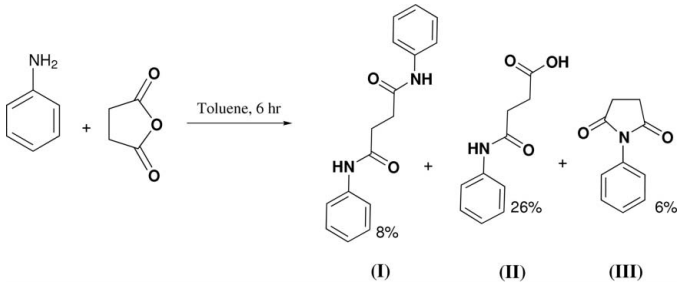
The title compound, $C_{16}H_{16}N_2O_2$, was synthesized by the condensation of aniline and succinic anhydride. The molecule lies across a crystallographic inversion centre. The dihedral angle between the benzene and acetamide planes is 33.36 (7)°. N—H···O hydrogen bonds link the molecules into chains along [010].

Comment

Methyl(2-methoxycarbonyl)succinate, a natural aromatic amide isolated from the methanolic extract of *Jolyna laminarioides*, has shown potent chymotrypsin inhibitory activity (Atta-ur-Rahman *et al.*, 1997). Therefore, we have synthesized our desired analogue (II), along with (I) and (III) as side products, by a one-step condensation of aniline and succinic anhydride (see scheme). The structural analogues of the title compound, (I), possess potent antifungal activity, especially against *Sclerotinia sclerotiorum* and *Botrytis cinerea* (Fujinami, Ozaki *et al.*, 1971; Fujinami, Tottori *et al.*, 1971; Fujinami *et al.*, 1972; Hisada *et al.*, 1976). We report here the structure of (I).



Molecules of the title compound, (I), lie across crystallographic inversion centres and the asymmetric unit therefore consists of one half-molecule (Fig. 1). Bond lengths and angles show normal values (Allen *et al.*, 1987). The succinamide moiety is not planar, as the inversion-related acetamide planes are stacked stepwise. The dihedral angle between the benzene

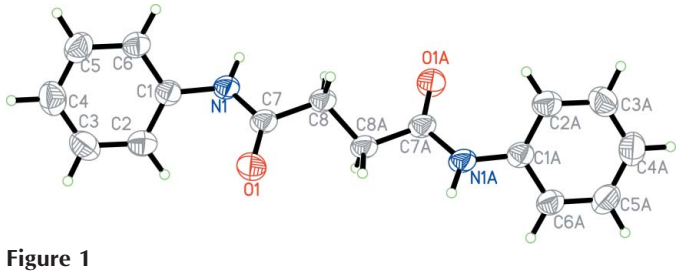


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The suffix A denotes an atom related by the symmetry operator $-x, 1-y, 1-z$.

and the acetamide planes is 33.36 (7)°. The N1—C7—C8 [114.45 (10)°] and C7—N1—C1 [126.69 (10)°] angles are comparable with the corresponding angles [112.90(17 and 125.19 (16)°] in *N*,*N*′-diphenylethylenediamine (Lennartson *et al.*, 2005).

The molecules are linked by intermolecular N—H···O hydrogen bonds (Table 1) to form chains along [010] (Fig.2).

Experimental

Succinic anhydride (1.06 g, 0.01 mol.) was added to aniline (5.6 ml, 0.06 mol) in a round-bottomed flask containing dry toluene (50 ml). The reaction mixture was then refluxed for 6 h using a Dean–Stark trap. The reaction mixture, a brownish gum containing three major compounds and weighing 2.03 g, was evaporated under vacuum and then purified by silica gel column chromatography using gradient elution with petroleum ether and chloroform. Colourless crystals of compound (I) (0.156 g, yield 8.0%, m.p. 539–540 K) were obtained on elution with petroleum ether and chloroform (2:3) (*Rf* = 0.3 in chloroform).

Crystal data

$C_{16}H_{16}N_2O_2$
M_r = 268.31
Monoclinic, $P2_1/c$
a = 6.6848 (9) Å
b = 5.1036 (7) Å
c = 19.596 (3) Å
β = 92.848 (2)°
V = 667.71 (16) Å^3
Z = 2
D_x = 1.335 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3999 reflections
θ = 2.1–26.0°
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, colourless
0.59 × 0.26 × 0.08 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.993
3465 measured reflections
1305 independent reflections
1170 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 26.0°
$h = -8 \rightarrow 8$
$k = -6 \rightarrow 5$
$l = -20 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.16
1305 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.0822P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.226 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	2.13	2.9699 (14)	165
C2—H2A···O1^{ii}	0.93	2.49	2.9359 (18)	109

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

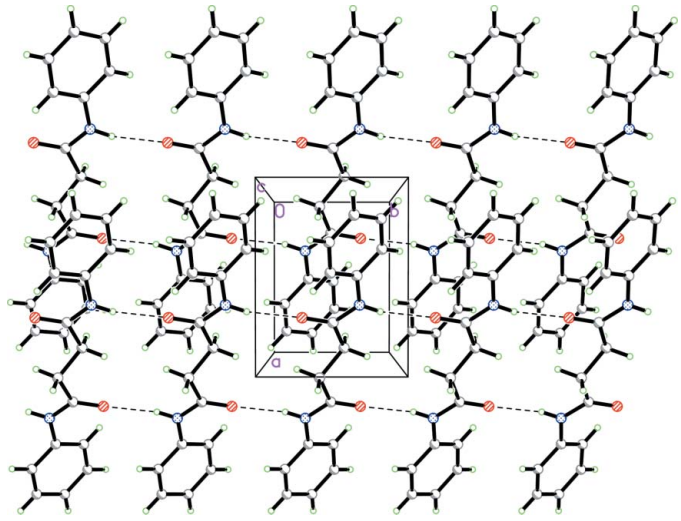


Figure 2
A view of the molecular packing in (I), viewed down the *c* axis. Dashed lines indicate hydrogen bonds.

H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H = 0.86 Å, C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C/N).

Data collection: *SMART* (Siemens, 1997); cell refinement: *SAINT* (Siemens, 1997); 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).

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