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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.035
wR factor = 0.094
Data-to-parameter ratio = 12.5

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

N-(2-Hydroxyphenyl)-N'-phenethylsuccinamide

Molecules of the title compound, $\text{C}_{18}\text{H}_{20}\text{N}_2\text{O}_3$, adopt a rod-like shape, probably influenced by $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds, which also determine the formation of polymeric chains along the glide direction.

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Comment

β -Phenylethylamide 2-hydroxisuccinanic acid (phensuccinal) is a novel prospective pharmacological agent which possesses antidiabetogenic effects due to the stimulation of pancreatic β -cell regeneration and to its antioxidant effect in animals with heterogeneous insulin insufficiency (Poltorack *et al.*, 1995). Knowledge of its molecular and crystal structure might be important in order to design other pharmaceutically acceptable forms.

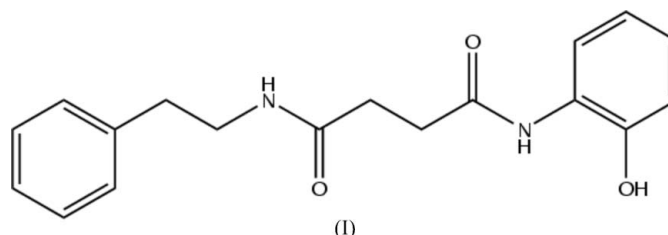
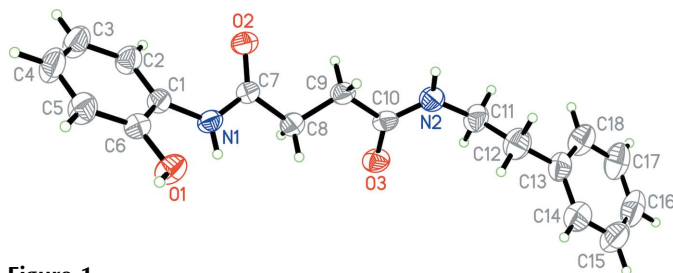


Fig. 1 shows a perspective view of the title molecule, (I). The central amide fragment and the C11 atom are coplanar within 0.01 \AA , in spite of the short intramolecular contact $\text{H9B}\cdots\text{H2N}$ [2.30 \AA ; sum of van der Waals radii is 2.34 \AA (Zefirov & Zorky, 1995)]. The methylenephanyl substituent at atom C11 is oriented almost orthogonal to the $\text{C10}-\text{N2}$ bond [the $\text{C10}-\text{N2}-\text{C11}-\text{C12}$ torsion angle is $-106.4 (2)^\circ$]. The phenyl substituent adopts an *ap* conformation relative to the $\text{C11}-\text{N2}$ bond [the $\text{N2}-\text{C11}-\text{C12}-\text{C13}$ torsion angle is $175.5 (2)^\circ$] and is twisted with respect to the $\text{C11}-\text{C12}$ bond [the $\text{C11}-\text{C12}-\text{C13}-\text{C18}$ torsion angle is $46.4 (2)^\circ$]. Such an orientation of the phenyl ring is caused by the repulsion between the C11 and C12 methylene groups and the atoms of the aromatic ring, as suggested by the short intramolecular contacts $\text{C11}\cdots\text{H18}$ (2.76 \AA ; sum of van der Waals radii 2.87 \AA), $\text{H11A}\cdots\text{C18}$ (2.80 \AA), $\text{H12A}\cdots\text{H14}$ (2.31 \AA ; sum of van der Waals radii 2.34 \AA), $\text{H11A}\cdots\text{H18}$ (2.32 \AA). The carbonyl groups of the two amide fragments are oriented in opposite directions and are twisted slightly with respect to the $\text{C8}-\text{C9}$ bond [the $\text{O2}-\text{C7}-\text{C8}-\text{C9}$ and $\text{O3}-\text{C10}-\text{C9}-\text{C8}$ torsion angles are $-176.0 (1)$ and $13.4 (2)^\circ$, respectively]. The hydroxyphenyl substituent has an *ap* orientation relative to the $\text{C8}-\text{C7}$ bond and is essentially non-coplanar with respect to the carbamide fragment [the $\text{C1}-\text{N1}-\text{C7}-\text{C8}$ and $\text{C7}-$


Figure 1

The molecular structure of the title compound. The non-H atoms are shown with displacement ellipsoids drawn at the 50% probability level.

N1—C1—C2 torsion angles are $-174.8(1)$ and $36.6(2)^\circ$, respectively]. This is probably caused by the short intramolecular contacts C7 \cdots H2 (2.85 Å; sum of van der Waals radii), O2 \cdots C2 (2.94 Å; sum of van der Waals radii 3.00 Å), H1N \cdots O1 (2.38 Å; sum of van der Waals radii 2.45 Å).

The molecules of the title compound form polymeric chains along the *c*-axis direction (Fig. 2) due to the formation of N—H \cdots O and O—H \cdots O intermolecular hydrogen bonds (Table 2). This, probably, results in an elongation of the N1—C7 and O3—C10 bonds (Table 1) compared with their mean values of 1.334 and 1.210 Å (Bürgi & Dunitz, 1994), respectively, and the shortening of the N2—C10 and N2—C11 bonds (mean values are 1.334 and 1.469 Å, respectively). Finally, there is a short intramolecular contact H1N \cdots H8B (2.21 Å; sum of van der Waals radii 2.34 Å). The formation of intermolecular hydrogen bonds is probably a stabilizing factor for the elongated rod-like shape of the molecules.

Experimental

The title compound was prepared according to Patent 36464 A Ukraine (2001). Crystals suitable for X-ray analysis were obtained by crystallization from isopropanol.

Crystal data

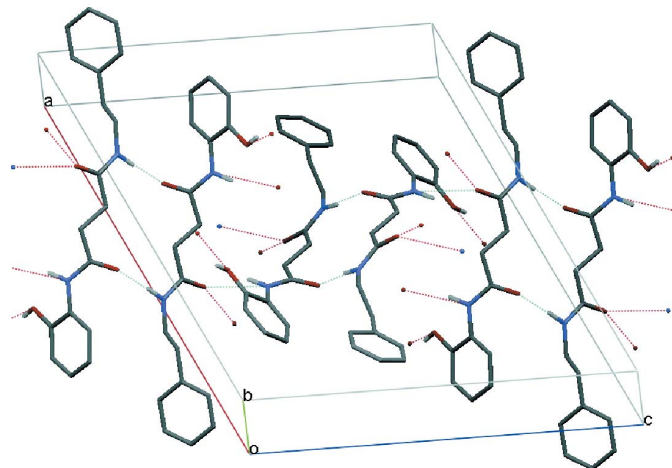
$C_{18}H_{20}N_2O_3$	$Z = 4$
$M_r = 312.36$	$D_x = 1.308 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 19.630(4) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 5.1128(8) \text{ \AA}$	$T = 293(2) \text{ K}$
$c = 17.326(4) \text{ \AA}$	Plate, colourless
$\beta = 114.17(2)^\circ$	$0.30 \times 0.20 \times 0.05 \text{ mm}$
$V = 1586.5(6) \text{ \AA}^3$	

Data collection

Oxford Diffraction Xcalibur-3 diffractometer	2755 independent reflections
ω scans	1954 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.019$
9600 measured reflections	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.035$	$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2]$
$wR(F^2) = 0.094$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2755 reflections	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
220 parameters	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$


Figure 2

Partial packing view of the structure, showing the hydrogen-bonded (dashed lines) polymeric chains.

Table 1

Selected bond lengths (Å).

N1—C7	1.3435 (18)	O1—C6	1.3551 (17)
N1—C1	1.4148 (18)	O2—C7	1.2246 (15)
N2—C10	1.3224 (19)	O3—C10	1.2428 (16)
N2—C11	1.4495 (19)	C7—C8	1.498 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N \cdots O3 ⁱ	0.816 (15)	2.224 (15)	2.9615 (17)	150.6 (13)
O1—H1O \cdots O3 ⁱⁱ	0.84 (2)	1.88 (2)	2.6648 (15)	156 (2)
N2—H2N \cdots O2 ⁱⁱⁱ	0.836 (16)	2.094 (17)	2.9254 (18)	173.0 (15)

Symmetry codes: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (ii) $-x + 1, y - \frac{3}{2}, -z + \frac{3}{2}$; (iii) $-x + 1, -y + 1, -z + 1$.

H atoms involved in hydrogen bonding were located in difference maps and refined with isotropic displacement factors [final N—H = 0.816 (15) and 0.836 (16) Å, and O—H = 0.84 (2) Å]; those attached to carbon were positioned geometrically (C—H = 0.93 or 0.97 Å) and allowed to ride, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve and refine structure: *SHELXTL* (Sheldrick, 1998); molecular graphics: *XP* (Siemens, 1998); software used to prepare material for publication: *SHELXTL*.

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