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4-Nitro-2-[(phenylhydrazono)methyl]phenol

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.150
Data-to-parameter ratio = 16.7

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

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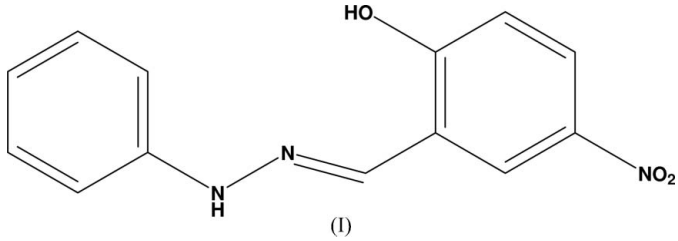
The molecular conformation of the title compound, $C_{13}H_{11}N_3O_3$, is stabilized by an intramolecular O—H···N hydrogen bond which generates an S(6) motif. The crystal packing is stabilized by N—H···O and C—H···O intermolecular interactions.

Comment

In supramolecular chemistry, the development of new receptors for anions has attracted much interest (Evans *et al.*, 2006). A general strategy for the production of a colorimetric sensor for anions is an anion-binding group with a chromogenic unit capable of signalling the binding event through an intramolecular charge-transfer process which leads to a change in colour visible to the naked eye (Suksai & Tuntulani, 2003). Aromatic nitro derivatives containing suitable binding groups have attracted more attention for selective and sensitive colorimetric detection of cations and anions (Kato *et al.*, 2001).



(I)

Bond lengths and bond angles in the title compound, (I), are comparable with literature values (Allen *et al.*, 1987). The torsion angles C3—C2—N1—O1 [−2.7 (2)°] and C1—C2—N1—O2 [−3.2 (2)°] indicate that the nitro group is almost coplanar with the benzene ring to which it is attached. The dihedral angle between the two benzene rings is 5.4 (1)°. The molecular conformation is stabilized by a strong O—H···N hydrogen bond, in which atom O3 acts as donor to N2, generating an S(6) motif. The crystal packing is stabilized by N—H···O and C—H···O intermolecular interactions (Table 1).

Experimental

The title compound was synthesized by Schiff base condensation between phenylhydrazine and 5-nitrosalicylaldehyde. Phenylhydrazine (0.5 ml, 4.62 mmol) in methanol (20 ml) was added to a solution of 5-nitrosalicylaldehyde (0.77 g, 4.62 mmol) in methanol (20 ml) with stirring. The solution was stirred for 1 h, and then heated to reflux for 30 min. The resulting solution was evaporated to obtain the product which was recrystallized from acetonitrile. Single crystals suitable for X-ray analysis were obtained by slow evaporation (yield 89%; m.p. 417 K).

Crystal data

$C_{13}H_{11}N_3O_3$
M_r = 257.25
Monoclinic, $P2_1/c$
a = 12.8167 (13) Å
b = 8.2176 (8) Å
c = 12.5848 (12) Å
β = 113.068 (2)°
V = 1219.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 273 (2) K
0.30 × 0.24 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
13440 measured reflections
2876 independent reflections
2440 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.150
S = 1.03
2876 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···N2	0.82	1.89	2.621 (1)	147
N3—H3A···O2^{i}	0.86	2.17	2.970 (2)	155
C1—H2···O3^{ii}	0.93	2.58	3.474 (1)	161

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

All H atoms were positioned geometrically (C—H = 0.93, N—H = 0.86 and O—H = 0.82 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C,N,O).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

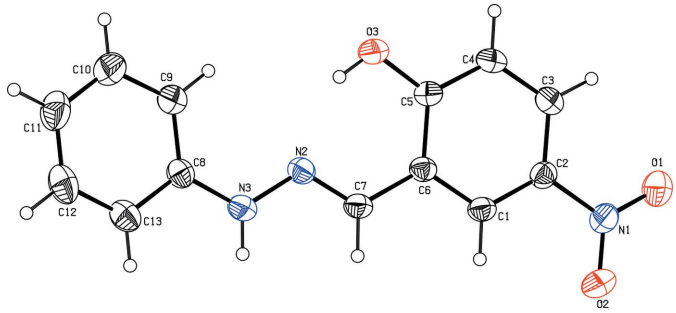


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

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