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3,5-Dimethyl-4-(2,4,6-trimethylphenyldiazenyl)phenol

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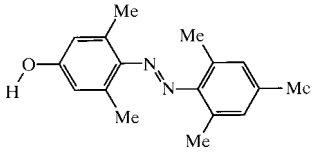
In the title compound, $C_{17}H_{20}N_2O$, (I), the dihedral angle between the two phenyl rings is 15.69 (6)°. An intermolecular hydrogen-bonding association exists between the hydroxy group and one of the azo N atoms.



(I)

Experimental

Crystals of the title compound were grown from ethyl acetate solution.

Crystal data

$C_{17}H_{20}N_2O$
M_r = 268.35
Monoclinic, $P2_1/n$
a = 12.369 (2) Å
b = 7.6809 (3) Å
c = 15.332 (3) Å
β = 101.842 (9)°
V = 1425.6 (4) Å^3
Z = 4
D_x = 1.250 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 6–14°
μ = 0.078 mm^{-1}
T = 298 (2) K
Block, red
0.47 × 0.47 × 0.47 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$2\theta/\omega$ scans
2679 measured reflections
2512 independent reflections
1717 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 24.97°
$h = -5 \rightarrow 14$
$k = -4 \rightarrow 9$
$l = -18 \rightarrow 17$
3 standard reflections every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.127
S = 1.034
2512 reflections
209 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 0.3065P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2^{i}	0.87 (3)	2.16 (3)	2.985 (2)	157 (2)

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

All H atoms were included in the refinement at calculated positions as riding models (C—H = 0.96 Å), except for the hydroxy H atom, which was located in difference syntheses and whose positional and displacement parameters were refined.

Data collection: *MolEN* (Fair, 1990); cell refinement: *MolEN*; data reduction: *Xtal*3.2 (Hall *et al.*, 1992); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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