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3-{(*E*)-[1-(2-Hydroxyphenyl)ethylidene]-amino}-1-(2-methylphenyl)thiourea

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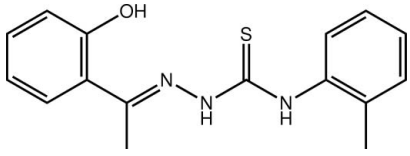
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.060; wR factor = 0.174; data-to-parameter ratio = 16.8.

In the title thiourea derivative, $C_{16}H_{17}N_3OS$, the hydroxy- and methyl-substituted benzene rings form dihedral angles of 9.62 (12) and 55.69 (6)°, respectively, with the central CN_3S chromophore (r.m.s. deviation = 0.0117 Å). An intramolecular O—H···N hydrogen bond ensures the coplanarity of the central atoms. The H atoms of the NH groups are *syn* and the conformation about the N=C double bond [1.295 (4) Å] is *E*. In the crystal, helical supramolecular chains sustained primarily by N—H···S hydrogen bonds are found. Additional stabilization is provided by C—H···π and π–π [ring centroid(hydroxybenzene)···ring centroid(methylbenzene) = 3.8524 (18) Å] interactions.

Related literature

For pharmaceutical applications of thioruea derivatives, see: Venkatachalam *et al.* (2004); Bruce *et al.* (2007). For related thiourea structures, see: Normaya *et al.* (2011); Salam *et al.* (2011); Dzulkifli *et al.* (2011).



Experimental

Crystal data

$C_{16}H_{17}N_3OS$
M_r = 299.39
Monoclinic, $P2_1/c$
a = 14.6966 (8) Å
b = 7.3586 (4) Å
c = 14.0926 (8) Å
β = 94.358 (5)°
V = 1519.66 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 100 K
0.30 × 0.10 × 0.05 mm

Data collection

Agilent Supernova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.419, T_{max} = 1.000
7614 measured reflections
3375 independent reflections
2094 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.174
S = 1.00
3375 reflections
201 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

*Cg*1 is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···N1	0.84 (1)	1.81 (2)	2.551 (3)	145 (3)
N2—H2n···S1^{i}	0.88 (1)	2.51 (2)	3.323 (2)	154 (3)
N3—H3n···S1^{i}	0.88 (1)	2.49 (2)	3.286 (3)	151 (2)
C8—H8b···*Cg*1^{i}	0.98	2.59	3.501 (3)	155

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5025).

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