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**Key indicators**  
Single-crystal X-ray study  
$T = 295$ K  
Mean $\sigma$(C–C) = 0.003 Å  
$R$ factor = 0.042  
w$R$ factor = 0.132  
Data-to-parameter ratio = 16.0  
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Molecules of the title compound, C$_{16}$H$_{16}$N$_2$O$_3$S, are linked by N—H···S hydrogen bonds to form centrosymmetric dimers [N···S = 3.4501 (13) Å]. The $N'$-phenyl and $N$-phenyl rings are twisted by 52.7 (1) and 23.3 (1)$^\circ$, respectively, from the essentially planar $-\text{NHC}(\equiv\text{S})\text{NC}(\equiv\text{O})-$ moiety.

**Comment**  
The crystal structures of a number of aromatic thioureas have been determined; the parent compound $N$-benzoyl-$N'$-phenylthiourea exists as a weakly held dimer arising from N—H···S interactions [N···S = 3.654 (1) Å; Yamin & Yusuf, 2003]. A non-planar conformation is adopted by the homolog having an electron-donating methoxy substituent in the $N'$-phenyl ring [N···S = 3.507 (3) Å; Cao et al., 1996].

![Figure 1](image_url)  
**Figure 1**  
ORTEPII plot (Johnson, 1976) of the title compound depicted as a centrosymmetric hydrogen-bonded dimer. Hydrogen bonds are shown as dashed lines, displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Unlabeled atoms are related by the symmetry code $(1 − x, 1 − y, 1 − z)$.
molecules are linked through N—H···S hydrogen bonds to form centrosymmetric dimers \([\text{N2} \cdots \text{S1}^i = 3.4501 (13) \, \text{Å}, \text{H2n} \cdots \text{S1}^i = 2.629 (16) \, \text{Å} \text{ and N2} \cdots \text{H2n} \cdots \text{S1}^i = 164 (2) \text{°};\) symmetry code: (i) \(1 – x, 1 – y, 1 – z\). The bond distances in the title compound are similar to those found in related systems (Yamin & Yusuf, 2003).

**Experimental**

An acetone solution of ammonium thiocyanate (0.50 g, 6.57 mmol) and 4-anisoyl chloride (1.12 g, 6.57 mmol) was vigorously stirred. To the solution was added 4-anisidine (0.80 g, 6.57 mmol) and the mixture was heated for 2 h. The solution when cooled yielded a brown precipitate; the crude compound was purified by recrystallization from ethyl acetate to give colorless crystals.

**Crystal data**

\(\text{C}_{16}\text{H}_{16}\text{N}_{2}\text{O}_{3}\text{S}\)

Monoclinic, \(P2_1/c\)

\(a = 11.4198 (7) \, \text{Å}\)

\(b = 11.0121 (7) \, \text{Å}\)

\(c = 12.2262 (8) \, \text{Å}\)

\(\beta = 93.319 (1)\)

\(V = 1534.94 (17) \, \text{Å}^3\)

\(Z = 4\)

\(D_x = 1.369 \, \text{Mg m}^{-3}\)

\(\mu = 0.23 \, \text{mm}^{-1}\)

\(\theta = 2.5–26.8^\circ\)

\(T = 295 (2) \, \text{K}\)

Data collection

Bruker SMART area-detector diffractometer

\(\phi\) and \(\omega\) scans

Absorption correction: none

2369 reflections with \(I > 2\sigma(I)\)

Refinement

Refinement on \(F^2\)

\(R[F^2 > 2\sigma(F^2)] = 0.042\)

\(wR(F^2) = 0.132\)

\(S = 1.03\)

3338 reflections

209 parameters

Carbon-bound H atoms were placed at calculated positions (C—H = 0.93 Å for the aromatic H atoms and C—H = 0.96 Å for the methyl H atoms) and were included in the refinement in the riding-model approximation, with \(U_{\text{iso}} = 1.2U_{eq}(C)\) for the aromatic H atoms and \(U_{\text{iso}} = 1.5U_{eq}(C)\) for the methyl H atoms. The torsion angle of the methyl groups was refined. Nitrogen-bound H atoms were located in a difference Fourier map and were refined with an N—H = 0.86 (1) Å distance restraint.

Data collection: \textit{SMART} (Bruker, 2001); cell refinement: \textit{SAINT} (Bruker, 2001); data reduction: \textit{SAINT}; program(s) used to solve structure: \textit{SHELXS97} (Sheldrick, 1997); program(s) used to refine structure: \textit{SHELXL97} (Sheldrick, 1997); molecular graphics: \textit{ORTEPII} (Johnson, 1976); software used to prepare material for publication: \textit{SHELXL97}.

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**References**


