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5-(3-Methylphenoxymethyl)-4-phenyl-1,2,4-triazole-3-thione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.098
Data-to-parameter ratio = 15.0

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

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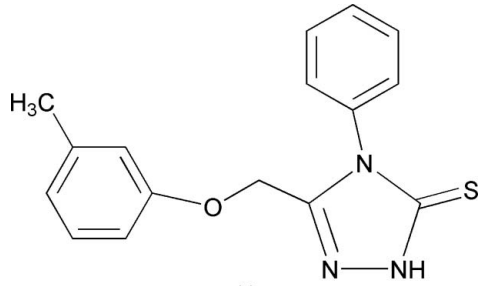
In the title compound, $C_{16}H_{15}N_3OS$, molecules form inversion-related dimers *via* N—H···S hydrogen bonds. The structure is further stabilized by intermolecular π–π stacking interactions down the *a* axis.

Comment

Substituted triazole derivatives display significant biological activity including antimicrobial (Holla *et al.*, 1998), analgesic (Turan-Zitouni *et al.*, 1999), antitumor (Demirbas *et al.*, 2002), antihypertensive (Paulvannan *et al.*, 2000) and antiviral activities (Kritsanida *et al.*, 2002). The biological activity is closely related to the structure, possibly being due to the presence of the —N—C═S unit (Omar *et al.*, 1986). We are interested in the synthesis and biological activity of aryloxyacetyl hydrazide derivatives and report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).



(I)

Compound (I) contains a planar triazolethione ring (mean deviation from the ring plane = 0.0008 Å). The dihedral angle between the C11–C16 phenyl ring and the triazole ring is 72.6 (2)°. In the crystal structure, molecules are linked into inversion-related dimers in the *ac* plane by N—H···S hydrogen bonds (Table 1 and Fig. 2).

The C11–C16 and C11^{i}—C16^{i} phenyl rings [symmetry code: (i) $2-x, -y, 1-z$] are parallel by symmetry, with a centroid–centroid distance of 4.070 Å. They thus form slipped-parallel dimers (Tsuzuki *et al.*, 2002; Hobza *et al.*, 1996); these intermolecular π–π interactions further stabilize the structure.

Experimental

The synthesis of the title compound was carried out by refluxing a solution of 1-(3-methylphenoxyacetyl)-4-phenylthiosemicarbazide (10 mmol) in 2 *M* NaOH for 2 h. Colorless single crystals of (I) were obtained by slow evaporation of an ethanol solution over a period of about one week.

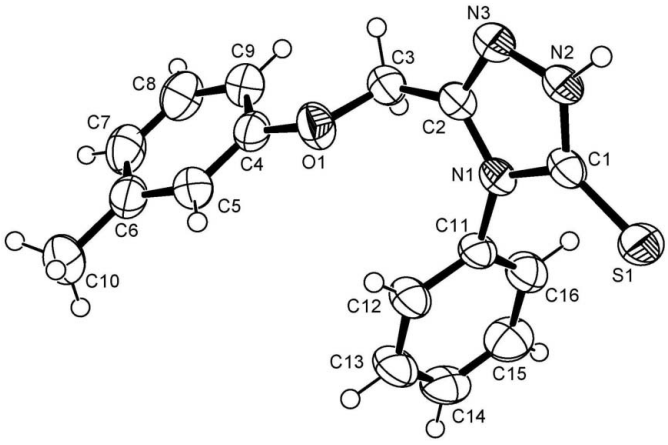


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

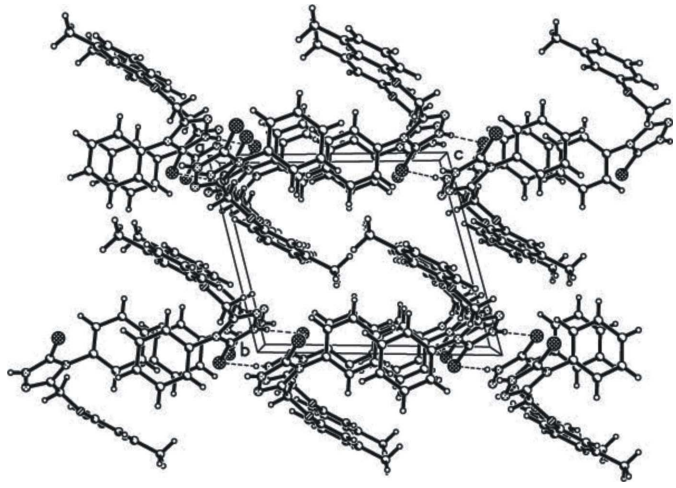


Figure 2
Packing diagram for (I), with hydrogen bonds shown as dashed lines.

Crystal data

$C_{16}H_{15}N_3OS$
M_r = 297.37
Triclinic, $P\overline{1}$
a = 6.9579 (12) Å
b = 9.8402 (18) Å
c = 11.686 (2) Å
α = 74.127 (3)°
β = 78.039 (3)°
γ = 82.196 (3)°
V = 750.2 (2) Å^3
Z = 2
D_x = 1.316 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 (2) K
Block, colorless
0.55 × 0.47 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.890, T_{max} = 0.934
6291 measured reflections
2920 independent reflections
2337 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.098
S = 1.03
2920 reflections
195 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.192P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···S1^{i}	0.86 (2)	2.40 (2)	3.2588 (14)	176.6 (17)

Symmetry code: (i) $-x+3, -y, -z$.

The N-bound H atom was located in a difference Fourier map and refined freely, with an isotropic displacement parameter. All other H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined using a riding model, with U_{iso}(H) = 1.5U_{eq}(methyl C) and 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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