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3-Benzyl-5-benzylidene-2-sulfanylidene-1,3-thiazolidin-4-one

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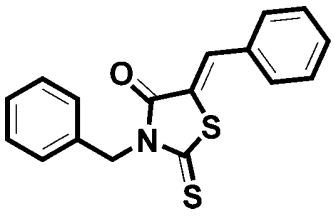
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.101; data-to-parameter ratio = 18.9.

In the title molecule, $C_{17}H_{13}NOS_2$, the essentially planar thiazole ring (r.m.s deviation 0.005 Å) forms dihedral angles of 16.85 (8)° and 75.02 (8)° with the phenyl rings. The dihedral angle between the two phenyl rings is 61.95 (9)°.

Related literature

For the synthesis and related structures, see: Shahwar *et al.* (2009, 2011).



Experimental

Crystal data

$C_{17}H_{13}NOS_2$
M_r = 311.40
Triclinic, $P\overline{1}$
a = 6.3152 (2) Å
b = 10.8168 (3) Å
c = 11.4545 (3) Å
α = 84.1150 (9)°
β = 77.6000 (9)°
γ = 76.1770 (9)°
V = 740.99 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 296 K
0.35 × 0.31 × 0.15 mm

Data collection

Bruker Kappa APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.886, T_{max} = 0.949
13205 measured reflections
3583 independent reflections
2930 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.03
3583 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5281).

References

Bruker (2007). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Shahwar, D., Tahir, M. N., Raza, M. A., Ahmad, N. & Aslam, S. (2011). *Acta Cryst.* E**67**, o133.
Shahwar, D., Tahir, M. N., Raza, M. A. & Iqbal, B. (2009). *Acta Cryst.* E**65**, o2917.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.