Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,3-Diphenylthiazolidin-5-amine

Jian-Gang Wang,[a] Fang-Fang Jian,[b]* Rui-Rui Zhuang[b] and Guang-Qiang Zhao[a]

[a]Bioengineering School, Weifang University, Weifang 261061, People's Republic of China, and [b]New Materials and Functional Coordination Chemistry Laboratory, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China

Correspondence e-mail: ffj2003@163169.net

Received 8 November 2006
Accepted 27 November 2006

Key indicators

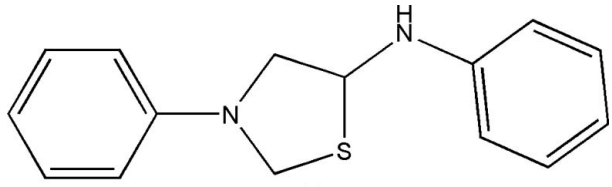
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.077
wR factor = 0.152
Data-to-parameter ratio = 14.0

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

The title compound, $C_{15}H_{14}N_2S$, was prepared by the reaction of aniline with isothiocanatobenzene and 1,2-dibromoethane at room temperature. The thiazolidne plane forms dihedral angles with the phenyl rings of 65.46 and 42.12°.

Comment

Heterocyclic compounds have fungicidal (Baker *et al.*, 2006) and pharmacological applications (Frydenvang *et al.*, 1997) together with wide use in pesticide production (Khalaf *et al.*, 2004). We report here the preparation and structure of a thiazolidine derivative, (I) (Fig. 1).



(I)

Bond lengths and angles in (I) are similar to those reported for this type of compound (Ji *et al.*, 2002). Atoms S1, N2, C7, C8 and C9 define the thiazolidne plane and the dihedral angles formed by the thiazolidne plane with the C1–C6 and C10–C15 phenyl rings are 65.46 and 42.12°, respectively. The C1–C6 and C10–C15 phenyl rings are inclined to one another at 48.06 (1)°. The bond distances S1—C7, S1—C9, N2—C7 and N2—C8 are 1.787, 1.802 ,1.385 and 1.464 Å respectively. The C1–C6 and C10–C15 phenyl rings are inclined to one another at 48.06 (1)°.

Experimental

A mixture of aniline (0.02 mol) and isothiocanatobenzene (0.02 mol) was stirred in dimethyl sulfoxide (30 ml) for 1.5 h. 1,2-Dibromo-

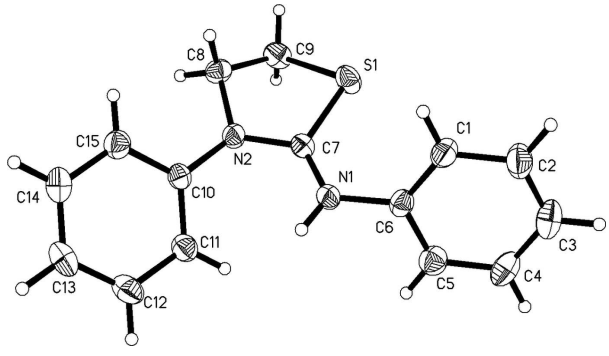


Figure 1
The molecular structure and atom-labelling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

ethane (0.02 mol) was added and the mixture stirred at 293 K for 1.5 h to afford the title compound (3.65 g, yield 51%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_{15}H_{15}N_2S$
M_r = 255.35
Monoclinic, $P2_1/c$
a = 10.742 (2) Å
b = 11.557 (2) Å
c = 10.568 (2) Å
β = 93.43 (3)°
V = 1309.6 (4) Å^3
Z = 4
D_x = 1.295 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 293 (2) K
Block, colourless
0.23 × 0.20 × 0.18 mm

Data collection

Enraf-Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
5203 measured reflections
2282 independent reflections
2170 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.152
S = 1.33
2282 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0273P)^2 + 1.3498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H and C—H distances of 0.86 and 0.93–0.96 Å, respectively, and with U_{iso}(H) = 1.2 or 1.5U_{eq} of the parent atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the Natural Science Foundation of Shandong Province (grant No. Y2005B04).

References

Baker, M. V., Barnard, P. J., Berners-Price, S. J., Brayshaw, S. K., Hickey, J. L., Skelton, B. W. & White, A. H. (2006). *Dalton Trans.* pp. 3708–3715.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Frydenvang, K., Matzen, L., Norrby, P. O., Slok, F. A., Liljefors, T., Krogsgaard-Larsen, P. & Jaroszewski, J. W. (1997). *J. Chem. Soc. Perkin Trans. 2*, pp. 1783–1792.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
Ji, B. M., Du, C. X., Zhu, Y. & Wang, Y. (2002). *Chin. J. Struct. Chem.* **21**, 252–255.
Khalaf, A. I., Ebrahimabadi, A. H., Drummond, A. J., Anthony, N. G., Mackay, S. P., Suckling, C. J. & Waigh, R. D. (2004). *Org. Biomol. Chem.* **2**, 3119–3127.
Sheldrick, G. M. (1990). *SHELXTL/PC*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.