

3-(*p*-Nitrobenzyl)-1,3-thiazolidine-2,4-dione

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Key indicators

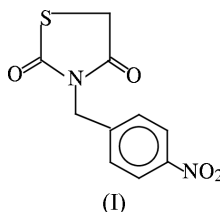
Single-crystal X-ray study
T = 173 K
Mean $\sigma(\text{C}-\text{C})$ = 0.004 Å
R factor = 0.048
wR factor = 0.123
Data-to-parameter ratio = 13.7

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

The title compound, C₁₀H₈N₂O₄S, serves as a starting material for the synthesis of antihyperglycemic pharmaceuticals. The nearly planar thiazolidine-2,4-dione ring is almost perpendicular to the nitrophenyl ring.

Comment

Thiazolidine-2,4-dione is used as a starting material for the synthesis of drugs with antihyperglycemic activity (Zask *et al.*, 1990). In heterocyclic chemistry, the thiazolidine-2,4-dione class is particularly important as a therapeutic agent and has been thoroughly investigated as a PPAR- γ -agonist that led to the development of several insulin-sensitizing drugs for the treatment of type-2 diabetes (Blanchet & Zhu, 2004). Diverse biological activities have been found to be associated with thiazolidine derivatives (Singh *et al.*, 1981). The present communication reports the synthesis of a novel thiazolidine-2,4-dione derivative, (I), and describes its crystal structure.



A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 1.6 plus three updates; *MOGUL* Version 1.0; Allen, 2002). The thiazolidine-2,4-dione ring is essentially planar (r.m.s. deviation 0.013 Å). It is almost perpendicular [89.67 (6)°] to the benzene ring. The nitro group is twisted by only 3.4 (6)° out of the plane of the benzene ring.

Experimental

An equimolar mixture of thiazolidine-2,4-dione (1.17 g, 10 mmol), 1-bromomethyl-4-nitrobenzene (2.16 g, 10 mmol) and anhydrous K₂CO₃ (1.38 g, 10 mmol) was stirred at room temperature in dimethylformamide (10 ml) for 6 h. The product formed was crystallized from methanol.

Crystal data

C₁₀H₈N₂O₄S
M_r = 252.24
Orthorhombic, *Pca*2₁
a = 24.321 (3) Å
b = 5.0468 (5) Å
c = 8.6066 (8) Å
V = 1056.40 (19) Å³
Z = 4
D_x = 1.586 Mg m⁻³

Mo *K*α radiation
Cell parameters from 8027 reflections
 θ = 2.7–26.1°
 μ = 0.31 mm⁻¹
T = 173 (2) K
Block, colourless
0.39 × 0.37 × 0.20 mm

Data collection

Stoe IPDS-II two-circle
diffractometer
 ω scans
Absorption correction: none
10054 measured reflections
2109 independent reflections

1895 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$
 $\theta_{\text{max}} = 26.2^\circ$
 $h = -30 \rightarrow 30$
 $k = -5 \rightarrow 6$
 $l = -10 \rightarrow 10$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.124$
 $S = 1.02$
2109 reflections
154 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.42 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.31 \text{ e } \text{\AA}^{-3}$
Absolute structure: Flack (1983),
971 Friedel pairs
Flack parameter = 0.03 (11)

Table 1

Selected bond lengths (\AA).

N1—C5	1.373 (4)	C2—S3	1.742 (3)
N1—C2	1.383 (3)	S3—C4	1.807 (3)
N1—C6	1.469 (3)	C4—C5	1.556 (3)

H atoms were geometrically positioned and refined with fixed individual displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$] using a riding model, with C—H = 0.99 and 0.95 \AA for methylene and aromatic CH groups, respectively.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine

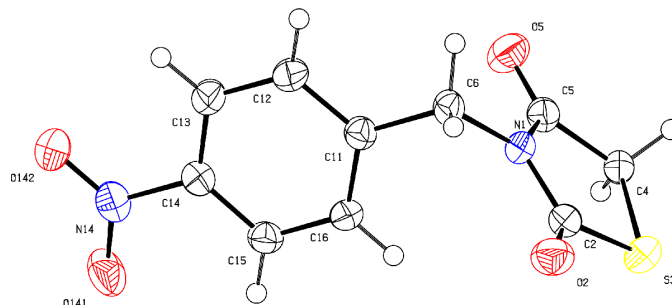


Figure 1

Perspective view of the title compound, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
- Blanchet, J. & Zhu, J. (2004). *Tetrahedron Lett.* **45**, 4449–4452.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Singh, S. P., Parmar, S. S., Raman, K. & Stenberg, V. I. (1981). *Chem. Rev.* **81**, 175–203.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
- Zask, A., Jirkovsky, I., Nowicki, J. W. & McCaleb, M. L. (1990). *J. Med. Chem.* **33**, 1418–1423.