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

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–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.

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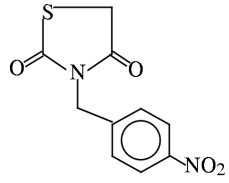
The title compound, $C_{10}H_8N_2O_4S$, serves as a starting material for the synthesis of antihyperglycemic pharmaceuticals. The nearly planar thiazolidine-2,4-dione ring is almost perpendicular to the nitrophenyl ring.

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.



(I)

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 K_2CO_3 (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

$C_{10}H_8N_2O_4S$
M_r = 252.24
Orthorhombic, $Pca2_1$
a = 24.321 (3) Å
b = 5.0468 (5) Å
c = 8.6066 (8) Å
V = 1056.40 (19) Å^3
Z = 4
D_x = 1.586 Mg m^{-3}
Mo $K\alpha$ 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 $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 26.2^{\circ}$
$h = -30 \rightarrow 30$
$k = -5 \rightarrow 6$
$l = -10 \rightarrow 10$

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

Table 1
Selected bond lengths (Å).

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_{iso}(H) = 1.2U_{eq}(C)] using a riding model, with C—H = 0.99 and 0.95 Å 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: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PLATON*.

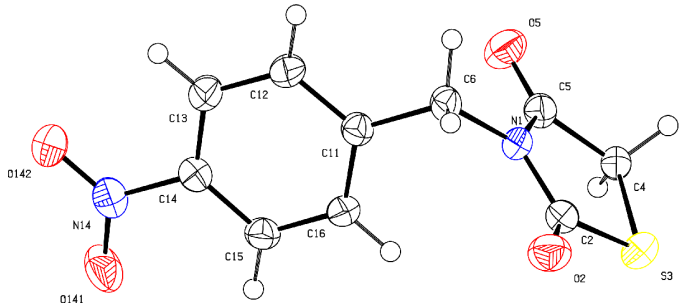


Figure 1
Perspective view of the title compound, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

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