

2-Imino-3-(2-nitrophenyl)-1,3-thiazolidin-4-one

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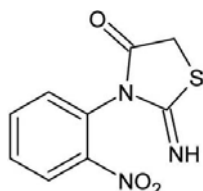
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.033; wR factor = 0.093; data-to-parameter ratio = 19.9.

In the title compound, $\text{C}_9\text{H}_7\text{N}_3\text{O}_3\text{S}$, the nitro and thiazolidinone moieties are inclined with respect to the aromatic ring at dihedral angles of 9.57 (16) and 78.42 (4)°, respectively. In the crystal, $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonding connects the molecules along the c and a axes to form a two-dimensional polymeric network. A weak $\text{S}\cdots\text{O}$ interaction [3.2443 (11) Å] and phenyl ring to phenyl ring off-set $\pi\cdots\pi$ stacking [with centroid-centroid separation of 3.6890 (7) Å and ring slippage of 1.479 Å] link the polymeric chains along the b and a axes, respectively.

Related literature

For the biological activities of thiazolidinones, see: Barreca *et al.* (2001); Shah & Desai (2007); Mehta *et al.* (2006); Vazzana *et al.* (2004); Wrobel *et al.* (2006). For related structures, see: Shahwar *et al.* (2009, 2011); Zhou *et al.* (2008). For graph-set notation, see: Bernstein *et al.* (1995). For the comparative C—C separation in graphite, see: Trucano & Chen (1975).



Experimental

Crystal data

$\text{C}_9\text{H}_7\text{N}_3\text{O}_3\text{S}$
 $M_r = 237.24$
 Monoclinic, $P2_1/n$

$a = 7.3036$ (5) Å
 $b = 16.4409$ (10) Å
 $c = 8.2455$ (5) Å

$\beta = 102.1321$ (9)°
 $V = 967.99$ (11) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.33$ mm⁻¹
 $T = 150$ K
 $0.70 \times 0.61 \times 0.40$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\text{min}} = 0.802$, $T_{\text{max}} = 0.880$

11000 measured reflections
 2938 independent reflections
 2675 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.093$
 $S = 1.03$
 2938 reflections
 148 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.47$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^{\text{i}}$	0.886 (18)	2.334 (18)	3.0337 (13)	135.9 (14)
$\text{N1}-\text{H1}\cdots\text{O2}^{\text{ii}}$	0.886 (18)	2.439 (17)	3.1416 (14)	136.5 (14)

Symmetry codes: (i) $x + 1, y, z$; (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$.

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: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2256).

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