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

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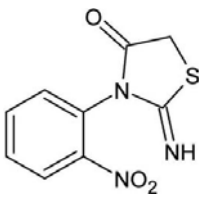
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.093; data-to-parameter ratio = 19.9.

In the title compound, $C_9H_7N_3O_3S$, 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, N—H···O hydrogen bonding connects the molecules along the c and a axes to form a two-dimensional polymeric network. A weak S···O interaction [3.2443 (11) Å] and phenyl ring to phenyl ring off-set π···π 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

$C_9H_7N_3O_3S$
M_r = 237.24
Monoclinic, $P2_1/n$
a = 7.3036 (5) Å
b = 16.4409 (10) Å
c = 8.2455 (5) Å
β = 102.1321 (9)°
V = 967.99 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 150 K
0.70 × 0.61 × 0.40 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.802, T_{max} = 0.880
11000 measured reflections
2938 independent reflections
2675 reflections with $I > 2\sigma(I)$
R_{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
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.886 (18)	2.334 (18)	3.0337 (13)	135.9 (14)
N1—H1···O2^{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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