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2-(4-Chlorophenyl)-3-*p*-tolyl-1,3-thiazolidin-4-one

Xiao-Jun Sun,* Jian-Feng Zhou, Zai-Chao Zhang and Yu-Jie Wang

Department of Chemistry, Huaiyin Teachers College, Huaian 223001, People's Republic of China
Correspondence e-mail: sunxiaojun100@126.com

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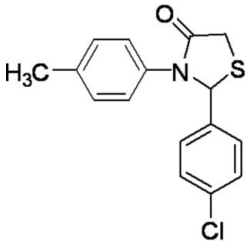
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.115; data-to-parameter ratio = 18.6.

The title compound, $C_{16}H_{14}ClNOS$, a potent antibacterial chemical, features a dihedral angle of 49.4 (1)° between the 4-tolyl and thiazolidinone rings, and a dihedral angle of 87.2 (5)° between the thiazolidinone and 4-chlorophenyl rings.

Related literature

For the synthesis, see: Srivastava *et al.* (2002).



Experimental

Crystal data

$C_{16}H_{14}ClNOS$ M_r = 303.79
Orthorhombic, *Pbca*
a = 12.1591 (4) Å
b = 13.0708 (4) Å
c = 18.5125 (7) Å
V = 2942.18 (17) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 296 K
0.40 × 0.35 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.85, T_{max} = 0.92
16959 measured reflections
3377 independent reflections
2205 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 1.02
3377 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2565).

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supporting information

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2-(4-Chlorophenyl)-3-*p*-tolyl-1,3-thiazolidin-4-one

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S1. Comment

4-thiazolidinone ring system comprises the broad spectrum for a number of biologically active compounds.In recent years, 4-thiazolidinones are the most extensively investigated class of compounds, which exhibits various biological activities, such as anticancer, antitubercular, antibacterial and herbicidal activities. In view of these properties and in a continuation of our interest in the chemistry of 4-thiazolidinones, we have attempted to synthesize a series of 4-thiazolidinone derivatives, some of which have comparatively high antibacterial activity. The crystal structure determination of the title compound,(I), was undertaken to investigate the relationship between structure and antibacterial activity(Fig. 1). The molecular conformation is described by the dihedral angle between 4-methylbenzene ring and thiazolidinone ring of 49.4 (1)° and the dihedral angle between thiazolidinone ring and 4-chlorobenzene ring of 87.2 (5)°.

S2. Experimental

Compound (I) was synthesized according to the procedure of Tumul Srivastava *et al.* (2002). A crystal of (I) suitable for X-ray analysis was grown from an ethanol solution by slow evaporation at room temperature.

S3. Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (aromatic), 0.99 (methylene), 1.00 (methylidyne) and 0.98 Å(methyl), and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

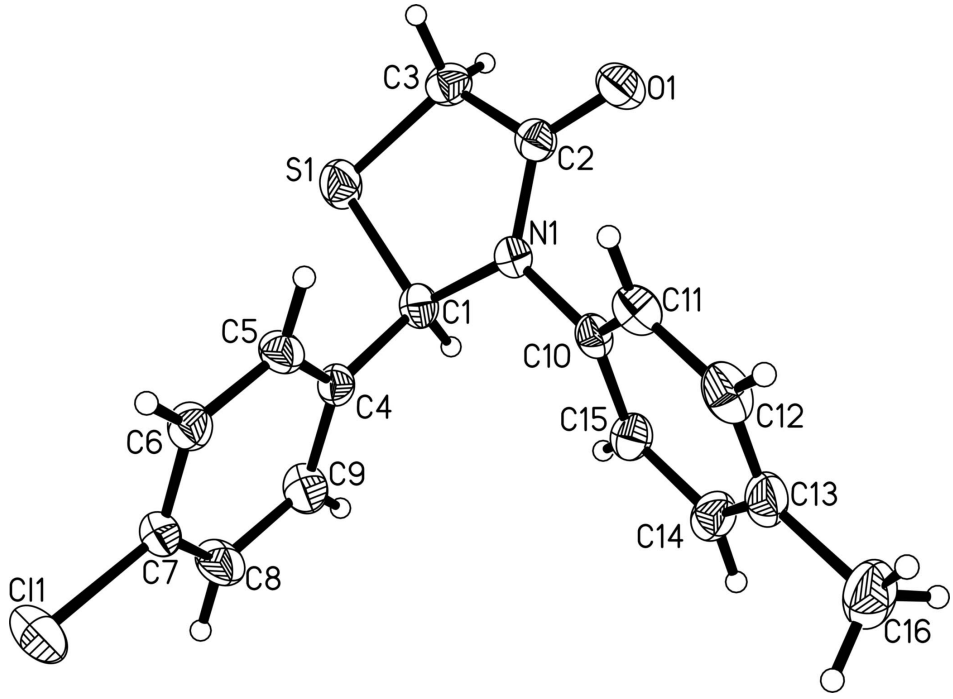

Figure 1

The molecular structure of (I), showing the atom-numbering schem. Displacement ellipsoids are drawn at the 30% probability level.

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Crystal data

$C_{16}H_{14}ClNOS$
$M_r = 303.79$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.1591\ (4)$ Å
$b = 13.0708\ (4)$ Å
$c = 18.5125\ (7)$ Å
$V = 2942.18\ (17)$ Å^3
$Z = 8$
$F(000) = 1264$
$D_x = 1.372$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2211 reflections
$\theta = 2.5–25.0°$
$\mu = 0.40$ mm^{-1}
$T = 296$ K
Plate, colorless
0.40 × 0.35 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
w\ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.85$, $T_{max} = 0.92$
16959 measured reflections
3377 independent reflections
2205 reflections with $I > 2\tilde{}I$)
$R_{int} = 0.058$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.2°$
$h = -14\rightarrow15$
$k = -16\rightarrow16$
$l = -24\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.115$
$S = 1.02$
3377 reflections
182 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 0.6312P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.66878 (17)	0.93240 (14)	0.34463 (11)	0.0402 (5)
H1	0.6105	0.9535	0.3112	0.048*
C2	0.85314 (18)	0.96718 (14)	0.30086 (12)	0.0399 (5)
C3	0.83681 (18)	1.05986 (15)	0.34764 (13)	0.0467 (6)
H3A	0.8310	1.1207	0.3179	0.056*
H3B	0.8990	1.0681	0.3800	0.056*
C4	0.62581 (16)	0.85053 (14)	0.39467 (11)	0.0368 (5)
C5	0.69556 (17)	0.79865 (16)	0.44122 (12)	0.0434 (5)
H5	0.7708	0.8112	0.4391	0.052*
C6	0.65582 (18)	0.72901 (15)	0.49046 (12)	0.0441 (5)
H6	0.7033	0.6949	0.5217	0.053*
C7	0.54441 (18)	0.71086 (15)	0.49257 (12)	0.0429 (5)
C8	0.47397 (18)	0.75886 (19)	0.44628 (14)	0.0546 (6)
H8	0.3990	0.7448	0.4478	0.065*
C9	0.51497 (18)	0.82863 (18)	0.39704 (13)	0.0508 (6)
H9	0.4673	0.8611	0.3652	0.061*
C10	0.76107 (17)	0.81131 (14)	0.25927 (11)	0.0380 (5)
C11	0.84795 (18)	0.74324 (15)	0.25858 (13)	0.0468 (5)
H11	0.9090	0.7546	0.2877	0.056*
C12	0.8436 (2)	0.65774 (16)	0.21407 (14)	0.0552 (6)
H12	0.9030	0.6130	0.2130	0.066*
C13	0.7532 (2)	0.63756 (16)	0.17140 (12)	0.0519 (6)
C14	0.6660 (2)	0.70546 (16)	0.17427 (12)	0.0510 (6)
H14	0.6037	0.6929	0.1465	0.061*
C15	0.66950 (18)	0.79175 (15)	0.21761 (12)	0.0433 (5)

H15	0.6101	0.8365	0.2186	0.052*
C16	0.7492 (3)	0.54493 (19)	0.12222 (16)	0.0780 (9)
H16A	0.8176	0.5085	0.1252	0.117*
H16B	0.7372	0.5668	0.0733	0.117*
H16C	0.6902	0.5008	0.1370	0.117*
Cl1	0.49492 (5)	0.62309 (5)	0.55527 (4)	0.0680 (2)
N1	0.76603 (13)	0.90125 (11)	0.30369 (9)	0.0371 (4)
O1	0.93527 (13)	0.95428 (11)	0.26448 (9)	0.0529 (4)
S1	0.71335 (6)	1.04265 (4)	0.39863 (3)	0.0568 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0406 (12)	0.0425 (11)	0.0373 (12)	0.0056 (9)	0.0029 (10)	0.0017 (9)
C2	0.0395 (12)	0.0439 (11)	0.0364 (12)	0.0001 (9)	−0.0021 (10)	0.0069 (9)
C3	0.0489 (13)	0.0427 (11)	0.0484 (14)	−0.0029 (9)	−0.0055 (11)	0.0022 (10)
C4	0.0358 (11)	0.0427 (10)	0.0319 (11)	0.0016 (8)	0.0025 (9)	−0.0025 (9)
C5	0.0305 (11)	0.0568 (12)	0.0429 (13)	−0.0040 (9)	−0.0001 (10)	0.0055 (10)
C6	0.0405 (13)	0.0533 (12)	0.0385 (13)	0.0006 (9)	−0.0027 (10)	0.0038 (10)
C7	0.0431 (13)	0.0470 (11)	0.0385 (12)	−0.0054 (9)	0.0083 (10)	−0.0005 (9)
C8	0.0306 (12)	0.0760 (15)	0.0571 (16)	−0.0067 (10)	0.0021 (11)	0.0084 (13)
C9	0.0403 (13)	0.0668 (14)	0.0452 (14)	0.0062 (10)	−0.0020 (11)	0.0077 (12)
C10	0.0431 (12)	0.0387 (10)	0.0322 (11)	−0.0010 (8)	0.0073 (10)	0.0046 (8)
C11	0.0419 (13)	0.0472 (11)	0.0512 (15)	0.0024 (9)	0.0064 (11)	0.0056 (10)
C12	0.0616 (16)	0.0423 (11)	0.0616 (17)	0.0112 (10)	0.0206 (14)	0.0076 (11)
C13	0.0736 (17)	0.0411 (11)	0.0409 (13)	−0.0031 (11)	0.0150 (13)	0.0008 (10)
C14	0.0659 (16)	0.0492 (12)	0.0379 (13)	−0.0041 (11)	−0.0044 (12)	0.0001 (10)
C15	0.0489 (13)	0.0429 (11)	0.0381 (12)	0.0045 (9)	−0.0015 (10)	0.0013 (9)
C16	0.120 (2)	0.0507 (14)	0.0634 (18)	0.0008 (15)	0.0190 (18)	−0.0083 (13)
Cl1	0.0592 (4)	0.0747 (4)	0.0701 (5)	−0.0107 (3)	0.0135 (3)	0.0234 (4)
N1	0.0368 (9)	0.0405 (8)	0.0339 (9)	−0.0006 (7)	0.0038 (8)	−0.0005 (7)
O1	0.0424 (9)	0.0556 (9)	0.0606 (11)	−0.0043 (7)	0.0109 (8)	0.0000 (8)
S1	0.0723 (5)	0.0469 (3)	0.0513 (4)	−0.0062 (3)	0.0169 (3)	−0.0087 (3)

Geometric parameters (Å, º)

C1—N1	1.462 (2)	C8—C9	1.382 (3)
C1—C4	1.509 (3)	C8—H8	0.9300
C1—S1	1.836 (2)	C9—H9	0.9300
C1—H1	0.9800	C10—C15	1.378 (3)
C2—O1	1.216 (2)	C10—C11	1.381 (3)
C2—N1	1.366 (3)	C10—N1	1.436 (2)
C2—C3	1.502 (3)	C11—C12	1.390 (3)
C3—S1	1.787 (2)	C11—H11	0.9300
C3—H3A	0.9700	C12—C13	1.378 (3)
C3—H3B	0.9700	C12—H12	0.9300
C4—C9	1.378 (3)	C13—C14	1.384 (3)
C4—C5	1.386 (3)	C13—C16	1.516 (3)

C5—C6	1.376 (3)	C14—C15	1.385 (3)
C5—H5	0.9300	C14—H14	0.9300
C6—C7	1.376 (3)	C15—H15	0.9300
C6—H6	0.9300	C16—H16A	0.9600
C7—C8	1.364 (3)	C16—H16B	0.9600
C7—Cl1	1.740 (2)	C16—H16C	0.9600
N1—C1—C4	113.63 (15)	C4—C9—H9	119.7
N1—C1—S1	105.19 (13)	C8—C9—H9	119.7
C4—C1—S1	108.94 (14)	C15—C10—C11	119.55 (19)
N1—C1—H1	109.6	C15—C10—N1	120.41 (18)
C4—C1—H1	109.6	C11—C10—N1	120.04 (19)
S1—C1—H1	109.6	C10—C11—C12	119.6 (2)
O1—C2—N1	124.76 (19)	C10—C11—H11	120.2
O1—C2—C3	122.66 (19)	C12—C11—H11	120.2
N1—C2—C3	112.58 (19)	C13—C12—C11	121.6 (2)
C2—C3—S1	108.30 (14)	C13—C12—H12	119.2
C2—C3—H3A	110.0	C11—C12—H12	119.2
S1—C3—H3A	110.0	C12—C13—C14	117.8 (2)
C2—C3—H3B	110.0	C12—C13—C16	121.6 (2)
S1—C3—H3B	110.0	C14—C13—C16	120.7 (3)
H3A—C3—H3B	108.4	C13—C14—C15	121.4 (2)
C9—C4—C5	118.47 (19)	C13—C14—H14	119.3
C9—C4—C1	120.36 (19)	C15—C14—H14	119.3
C5—C4—C1	121.12 (18)	C10—C15—C14	120.0 (2)
C6—C5—C4	121.38 (19)	C10—C15—H15	120.0
C6—C5—H5	119.3	C14—C15—H15	120.0
C4—C5—H5	119.3	C13—C16—H16A	109.5
C5—C6—C7	118.6 (2)	C13—C16—H16B	109.5
C5—C6—H6	120.7	H16A—C16—H16B	109.5
C7—C6—H6	120.7	C13—C16—H16C	109.5
C8—C7—C6	121.4 (2)	H16A—C16—H16C	109.5
C8—C7—Cl1	120.35 (17)	H16B—C16—H16C	109.5
C6—C7—Cl1	118.25 (17)	C2—N1—C10	121.80 (17)
C7—C8—C9	119.4 (2)	C2—N1—C1	118.11 (16)
C7—C8—H8	120.3	C10—N1—C1	119.39 (15)
C9—C8—H8	120.3	C3—S1—C1	93.39 (9)
C4—C9—C8	120.7 (2)		