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(*E*)-3-(4-Methylphenyl)-1-(1,3-thiazol-2-yl)prop-2-en-1-one

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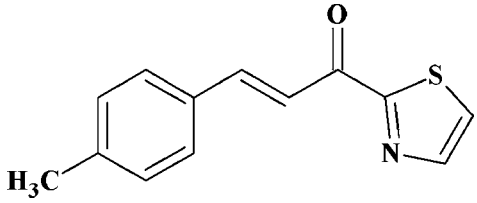
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.118; data-to-parameter ratio = 18.4.

In the title chalcone, $C_{13}H_{11}NOS$, derived from the condensation of *p*-tolualdehyde and 1-(1,3-thiazol-2-yl)ethanone, the olefine group has a *trans* configuration. No classical hydrogen bonding is present in the crystal structure.

Related literature

For background to thiazoles, see: Fontecave *et al.* (2003); Kleemann *et al.* (2001) and for their biological activity, see: Bharti *et al.* (2010); Bell *et al.* (1995); Cortes *et al.* (2007).



Experimental

Crystal data

$C_{13}H_{11}NOS$
M_r = 229.29
Monoclinic, $P2_1/c$
a = 13.9486 (9) Å
b = 11.1773 (8) Å
c = 7.4579 (5) Å
β = 102.061 (4)°
V = 1137.08 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.949, T_{max} = 0.949
10320 measured reflections
2808 independent reflections
2070 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.118
S = 1.05
2808 reflections
153 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2285).

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(*E*)-3-(4-Methylphenyl)-1-(1,3-thiazol-2-yl)prop-2-en-1-one

Annamalai Palaniappan, Arumugam Arulmozhivarman, Rajamanickam Ramachandran, Subramanian Srinivasan and Sivakolunthu Senthan

S1. Comment

Molecules which possess both sulphur and nitrogen atoms exhibit universal and crucial roles in living organisms (Fontecave *et al.*, 2003), with thiazoles and their derivatives being an important class of heterocyclic compounds (Kleemann *et al.*, 2001). Analogues of these are present in several drugs with a wide range of biological properties, such as antibacterial (Bharti *et al.*, 2010), antiviral (Bell *et al.*, 1995) and anticancer (Cortes *et al.*, 2007). Our research has been focused towards finding new therapeutic agents, using thiazole compounds. Similarly, several *α*,*β*-unsaturated ketones have been found to have good biological activity. Therefore, in this paper we report both the thiazole and *α*,*β*-unsaturated ketone moieties in one molecule. The title compound (Fig. 1) exists in an E configuration with respect to the C7-C8 double bond. Both phenyl and thiazole rings adopt planar orientations and there is no classical hydrogen bonding found.

S2. Experimental

To an aqueous ethanolic solution of p-tolualdehyde (0.01 mol) and 2-acetylthiazole (0.01 mol), a sodium hydroxide solution was added slowly and stirred until a precipitate formed. The obtained solid was filtered and washed well with water. Single crystals were grown by the slow evaporation technique using ethanol as solvent.

S3. Refinement

H-atoms were positioned and refined using a riding model, with aromatic C—H = 0.93 Å, methine C—H = 0.98 Å, methylene C—H = 0.97 Å and amino N—H = 0.83 and 0.94 Å. The displacement parameters were set for phenyl, methylene and aliphatic H atoms at U_{iso}(H)=1.2U_{eq}(C).

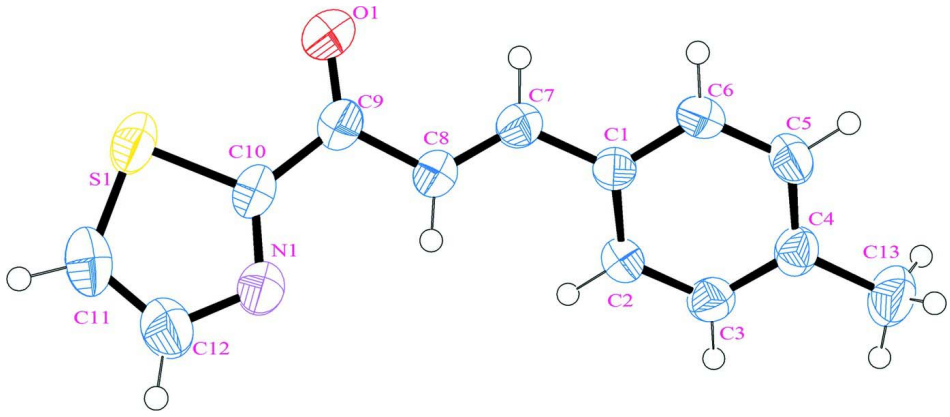

Figure 1

The *ORTEP* representation of title compound showing the atom numbering scheme and ellipsoids at the 50% probability level.

(*E*)-3-(4-Methylphenyl)-1-(1,3-thiazol-2-yl)prop-2-en-1-one

Crystal data

$C_{13}H_{11}NOS$
$M_r = 229.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.9486\ (9)$ Å
$b = 11.1773\ (8)$ Å
$c = 7.4579\ (5)$ Å
$\beta = 102.061\ (4)°$
$V = 1137.08\ (13)$ Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.339$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\mu = 0.26$ mm^{-1}
$T = 293$ K
Prism, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.949$, $T_{max} = 0.949$
10320 measured reflections
2808 independent reflections
2070 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.5°$
$h = -18\rightarrow17$
$k = -11\rightarrow14$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.118$
$S = 1.05$
2808 reflections
153 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.1832P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.98502 (3)	0.17057 (5)	1.16674 (6)	0.05963 (18)
O1	0.82353 (10)	−0.00430 (12)	1.0300 (2)	0.0721 (4)
N1	0.84607 (10)	0.31056 (13)	1.0198 (2)	0.0540 (4)
C1	0.53219 (10)	0.08303 (13)	0.72422 (19)	0.0380 (3)
C7	0.62986 (11)	0.05556 (15)	0.8309 (2)	0.0425 (3)
C4	0.34124 (11)	0.13769 (15)	0.5336 (2)	0.0451 (4)
C10	0.86817 (11)	0.19796 (15)	1.0453 (2)	0.0440 (4)
C2	0.51393 (11)	0.18190 (13)	0.6090 (2)	0.0420 (3)
H2	0.5657	0.2309	0.5948	0.050*
C8	0.70403 (11)	0.13124 (16)	0.8719 (2)	0.0471 (4)
C3	0.42049 (11)	0.20835 (15)	0.5155 (2)	0.0458 (4)
H3	0.4102	0.2748	0.4388	0.055*
C6	0.45308 (11)	0.01025 (14)	0.7382 (2)	0.0451 (4)
H6	0.4635	−0.0578	0.8113	0.054*
C9	0.79948 (11)	0.09785 (15)	0.9842 (2)	0.0476 (4)
C5	0.35920 (12)	0.03767 (15)	0.6448 (2)	0.0497 (4)
H5	0.3074	−0.0119	0.6570	0.060*
C13	0.23967 (13)	0.16866 (19)	0.4303 (3)	0.0681 (5)
H4C	0.2421	0.2405	0.3608	0.102*
H4A	0.1977	0.1809	0.5156	0.102*
H4B	0.2145	0.1043	0.3487	0.102*
C12	0.92396 (14)	0.37879 (19)	1.1005 (3)	0.0646 (5)
H12	0.9216	0.4619	1.0966	0.078*
C11	1.00462 (14)	0.31959 (19)	1.1861 (3)	0.0622 (5)
H11	1.0625	0.3554	1.2469	0.075*
H7	0.6378 (13)	−0.0218 (18)	0.877 (2)	0.059 (5)*
H8	0.6995 (14)	0.2095 (18)	0.835 (3)	0.066 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0395 (2)	0.0771 (4)	0.0562 (3)	0.0054 (2)	−0.00395 (18)	0.0080 (2)
O1	0.0545 (7)	0.0519 (8)	0.1003 (11)	0.0082 (6)	−0.0058 (7)	0.0108 (7)
N1	0.0422 (7)	0.0531 (9)	0.0628 (9)	0.0023 (6)	0.0019 (6)	−0.0033 (7)
C1	0.0372 (7)	0.0350 (7)	0.0417 (7)	0.0004 (6)	0.0080 (6)	−0.0042 (6)
C7	0.0412 (8)	0.0394 (8)	0.0465 (8)	0.0040 (6)	0.0079 (6)	−0.0002 (7)

C4	0.0383 (7)	0.0472 (9)	0.0476 (8)	0.0011 (6)	0.0040 (6)	−0.0089 (7)
C10	0.0333 (7)	0.0566 (9)	0.0405 (8)	0.0055 (7)	0.0041 (6)	0.0014 (7)
C2	0.0389 (7)	0.0395 (8)	0.0477 (8)	−0.0048 (6)	0.0096 (6)	0.0008 (6)
C8	0.0390 (8)	0.0444 (9)	0.0544 (9)	0.0022 (7)	0.0017 (7)	0.0025 (7)
C3	0.0469 (8)	0.0420 (8)	0.0465 (8)	0.0026 (7)	0.0046 (6)	0.0035 (7)
C6	0.0478 (8)	0.0341 (8)	0.0526 (9)	−0.0041 (6)	0.0083 (7)	0.0028 (7)
C9	0.0378 (7)	0.0517 (10)	0.0519 (9)	0.0049 (7)	0.0059 (6)	0.0019 (7)
C5	0.0410 (8)	0.0459 (9)	0.0619 (10)	−0.0110 (7)	0.0099 (7)	−0.0046 (7)
C13	0.0425 (9)	0.0759 (13)	0.0777 (13)	0.0042 (9)	−0.0063 (9)	−0.0058 (10)
C12	0.0560 (10)	0.0618 (12)	0.0722 (12)	−0.0096 (9)	0.0047 (9)	−0.0107 (10)
C11	0.0466 (9)	0.0835 (14)	0.0530 (10)	−0.0139 (9)	0.0025 (8)	−0.0082 (9)

Geometric parameters (Å, º)

S1—C11	1.689 (2)	C2—C3	1.376 (2)
S1—C10	1.7185 (15)	C2—H2	0.9300
O1—C9	1.219 (2)	C8—C9	1.465 (2)
N1—C10	1.300 (2)	C8—H8	0.92 (2)
N1—C12	1.360 (2)	C3—H3	0.9300
C1—C2	1.390 (2)	C6—C5	1.383 (2)
C1—C6	1.392 (2)	C6—H6	0.9300
C1—C7	1.460 (2)	C5—H5	0.9300
C7—C8	1.322 (2)	C13—H4C	0.9600
C7—H7	0.929 (19)	C13—H4A	0.9600
C4—C5	1.383 (2)	C13—H4B	0.9600
C4—C3	1.388 (2)	C12—C11	1.346 (3)
C4—C13	1.505 (2)	C12—H12	0.9300
C10—C9	1.482 (2)	C11—H11	0.9300
C11—S1—C10	89.32 (9)	C4—C3—H3	119.4
C10—N1—C12	109.56 (16)	C5—C6—C1	120.99 (14)
C2—C1—C6	117.70 (13)	C5—C6—H6	119.5
C2—C1—C7	122.26 (13)	C1—C6—H6	119.5
C6—C1—C7	120.03 (14)	O1—C9—C8	124.27 (16)
C8—C7—C1	126.00 (15)	O1—C9—C10	119.91 (15)
C8—C7—H7	118.9 (11)	C8—C9—C10	115.81 (14)
C1—C7—H7	115.1 (11)	C6—C5—C4	120.98 (14)
C5—C4—C3	118.03 (14)	C6—C5—H5	119.5
C5—C4—C13	121.73 (16)	C4—C5—H5	119.5
C3—C4—C13	120.21 (16)	C4—C13—H4C	109.5
N1—C10—C9	124.58 (14)	C4—C13—H4A	109.5
N1—C10—S1	114.79 (12)	H4C—C13—H4A	109.5
C9—C10—S1	120.58 (12)	C4—C13—H4B	109.5
C3—C2—C1	121.05 (14)	H4C—C13—H4B	109.5
C3—C2—H2	119.5	H4A—C13—H4B	109.5
C1—C2—H2	119.5	C11—C12—N1	116.45 (19)
C7—C8—C9	122.88 (16)	C11—C12—H12	121.8
C7—C8—H8	122.7 (12)	N1—C12—H12	121.8

C9—C8—H8	114.4 (13)	C12—C11—S1	109.87 (15)
C2—C3—C4	121.20 (15)	C12—C11—H11	125.1
C2—C3—H3	119.4	S1—C11—H11	125.1
C2—C1—C7—C8	19.2 (2)	C7—C1—C6—C5	177.01 (15)
C6—C1—C7—C8	−159.68 (16)	C7—C8—C9—O1	9.7 (3)
C12—N1—C10—C9	176.99 (16)	C7—C8—C9—C10	−169.19 (15)
C12—N1—C10—S1	−0.58 (19)	N1—C10—C9—O1	−172.68 (16)
C11—S1—C10—N1	0.65 (14)	S1—C10—C9—O1	4.8 (2)
C11—S1—C10—C9	−177.02 (14)	N1—C10—C9—C8	6.3 (2)
C6—C1—C2—C3	1.5 (2)	S1—C10—C9—C8	−176.29 (12)
C7—C1—C2—C3	−177.40 (14)	C1—C6—C5—C4	0.6 (2)
C1—C7—C8—C9	178.32 (14)	C3—C4—C5—C6	1.3 (2)
C1—C2—C3—C4	0.3 (2)	C13—C4—C5—C6	179.72 (16)
C5—C4—C3—C2	−1.7 (2)	C10—N1—C12—C11	0.2 (2)
C13—C4—C3—C2	179.84 (16)	N1—C12—C11—S1	0.3 (2)
C2—C1—C6—C5	−2.0 (2)	C10—S1—C11—C12	−0.52 (15)