Atomic coordinates are in Table 1.* A perspective molecular drawing and the atomic labelling scheme are displayed in Fig. 1. Bond distances and angles are listed in Table 2.

Related literature. The title compound was prepared in connection with our studies on the protonation sites of organic bases with several nitrogen functions (Soriano-García, Toscano & Espinosa, 1985; Soriano-García, Toscano & Schatz-Levine, 1987).

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52594 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of Ethyl 2-Acetyl-3-[5-(*p*-tolyl)-2-furyl]acrylate

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Abstract. $C_{18}H_{18}O_4$, $M_r = 298{\cdot}3$, orthorhombic, *Pbca*, $a = 7{\cdot}519\ (1)$, $b = 21{\cdot}926\ (6)$, $c = 19{\cdot}134\ (4)$ Å, $V = 3154{\cdot}5$ Å^3, $Z = 8$, $D_m = 1{\cdot}24$, $D_x = 1{\cdot}256$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 0{\cdot}68$ mm^{-1}, $F(000) = 1264$, $T = 293$ K, final $R = 0{\cdot}052$ for 1890 unique observed reflections. There is extensive π delocalization involving the phenyl, furyl and acetylethylenic groups as shown by the pattern of bond lengths and the planarity of the system (the phenyl/furyl and acetylethylenic group/furyl dihedral angles are 1·3 and 1·0°, respectively) while the ethoxycarbonyl moiety is nearly perpendicular to the conjugated system (dihedral angle 91·5°). The molecules are held together by van der Waals forces only.

Experimental. Transparent prism-like crystal of dimensions 0·1 × 0·15 × 0·75 mm; D_m by flotation in bromoform/*n*-octane; systematic absences: 0*kl* for *k* odd, *h*0*l* for *l* odd and *hk*0 for *h* odd; Syntex $P2_1$ diffractometer, graphite-monochromated Cu $K\alpha$ radiation; room temperature; choice of unit-cell parameters verified by *UB* (Sivý, Sivý & Koreň, 1987), refinement on the basis of 15 reflections, $10 < \theta < 25°$; intensity data ($h = 0$ to 8, $k = 0$ to 25, $l = 0$ to 22) by $\theta/2\theta$ scans, $2\theta \leq 130°$; three standards measured every 100 reflections, no significant systematic fluctuation; 2682 unique reflections, 1890 with $I \geq 2\sigma(I)$ considered observed and included in the refinement; data reduction using *XP*21 (Pavelčík,

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Table 1. *Final atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (4/3)\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
C(1)	2328 (2)	2364 (1)	−671 (1)	5·53
C(2)	2483 (2)	2720 (1)	1 (1)	4·42
C(3)	3046 (2)	3325 (1)	0 (1)	4·54
C(4)	3165 (2)	3656 (1)	611 (1)	4·40
C(5)	2726 (2)	3392 (1)	1252 (1)	3·94
C(6)	2153 (2)	2789 (1)	1256 (1)	4·68
C(7)	2043 (2)	2460 (1)	640 (1)	4·83
C(8)	2830 (1)	3734 (1)	1902 (1)	4·22
O(9)	3356 (1)	4331 (0)	1853 (0)	4·12
C(10)	3378 (2)	4565 (1)	2519 (1)	4·45
C(11)	2848 (2)	4125 (1)	2973 (1)	5·73
C(12)	2517 (2)	3596 (1)	2586 (1)	5·56
C(13)	3871 (2)	5187 (1)	2621 (1)	4·46
C(14)	4352 (2)	5601 (1)	2138 (1)	3·89
C(15)	4805 (2)	6237 (1)	2305 (1)	4·35
O(16)	5209 (1)	6583 (0)	1829 (1)	5·96
C(17)	4791 (2)	6459 (1)	3049 (1)	5·47
C(18)	4429 (2)	5468 (1)	1371 (1)	4·03
O(19)	5722 (1)	5302 (0)	1056 (0)	5·12
O(20)	2856 (1)	5583 (0)	1074 (0)	4·60
C(21)	2737 (2)	5524 (1)	315 (1)	5·30
C(22)	941 (2)	5766 (1)	115 (1)	6·19

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(1)—C(2)	1·509 (2)	C(12)—C(8)	1·363 (2)
C(2)—C(3)	1·392 (2)	C(10)—C(13)	1·426 (2)
C(3)—C(4)	1·379 (2)	C(13)—C(14)	1·345 (2)
C(4)—C(5)	1·395 (2)	C(14)—C(15)	1·472 (2)
C(5)—C(6)	1·390 (2)	C(15)—O(16)	1·223 (2)
C(6)—C(7)	1·385 (2)	C(15)—C(17)	1·504 (2)
C(7)—C(2)	1·389 (2)	C(14)—C(18)	1·497 (2)
C(5)—C(8)	1·453 (2)	C(18)—O(19)	1·200 (2)
C(8)—O(9)	1·371 (2)	C(18)—O(20)	1·336 (2)
O(9)—C(10)	1·374 (2)	O(20)—C(21)	1·460 (2)
C(10)—C(11)	1·357 (2)	C(21)—C(22)	1·500 (2)
C(11)—C(12)	1·399 (2)		

C(1)—C(2)—C(3)	121·0 (1)	C(10)—C(13)—C(14)	128·4 (1)
C(1)—C(2)—C(7)	121·2 (1)	C(13)—C(14)—C(15)	123·6 (1)
C(3)—C(2)—C(7)	117·7 (1)	C(13)—C(14)—C(18)	123·5 (1)
C(2)—C(3)—C(4)	121·3 (1)	C(15)—C(14)—C(18)	112·9 (1)
C(3)—C(4)—C(5)	120·8 (1)	C(14)—C(15)—O(16)	118·9 (1)
C(4)—C(5)—C(6)	118·1 (1)	C(14)—C(15)—C(17)	120·7 (1)
C(4)—C(5)—C(8)	121·7 (1)	O(16)—C(15)—C(17)	120·4 (1)
C(6)—C(5)—C(8)	120·1 (1)	C(14)—C(18)—O(19)	125·6 (1)
C(5)—C(8)—O(9)	116·7 (1)	C(14)—C(18)—O(20)	110·2 (1)
C(5)—C(8)—C(12)	134·3 (1)	O(19)—C(18)—O(20)	124·1 (1)
O(9)—C(8)—C(12)	109·0 (1)	C(18)—O(20)—C(21)	117·4 (1)
C(8)—O(9)—C(10)	107·3 (1)	O(20)—C(21)—C(22)	106·2 (1)
O(9)—C(10)—C(11)	108·9 (1)	C(5)—C(6)—C(7)	120·7 (1)
O(9)—C(10)—C(13)	119·1 (1)	C(2)—C(7)—C(6)	121·3 (1)
C(11)—C(10)—C(13)	131·9 (1)	C(10)—C(11)—C(12)	107·6 (1)
		C(8)—C(12)—C(11)	107·2 (1)

1987); structure solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and *MAGEX* (Hull, Viterbo, Woolfson & Zhang, 1981) and refined by block-diagonal least squares; $\Delta\rho$ map showed positions of all H atoms, refinement continued on positional parameters, anisotropic displacement parameters for non-H atoms and isotropic displacement parameters for H atoms; in final cycle $R = 0{\cdot}052$, $wR = 0{\cdot}059$ for observed reflections only, $S = 1{\cdot}6$, max. shift/e.s.d. 0·12, function minimized $\sum w(\Delta F)^2$, where $w = 1$ if $|F_o| < 30$ and $w = 30/|F_o|$ if $|F_o| \geq 30$, max. and min. heights in final $\Delta\rho$ synthesis 0·40 and −0·25 e Å^{-3}, scattering factors from *International Tables for X-ray Crystallography* (1974); all calculations except *UB*, *XP*21, *MULTAN* and *MAGEX* performed with a local version of the *NRC* system (Ahmed, Hall, Pippy & Huber, 1973). Final atomic coordinates of non-H atoms and equivalent isotropic B's are listed in Table 1,* bond distances and angles in Table 2. A perspective drawing of the molecule and numbering of the atoms are shown in Fig. 1.

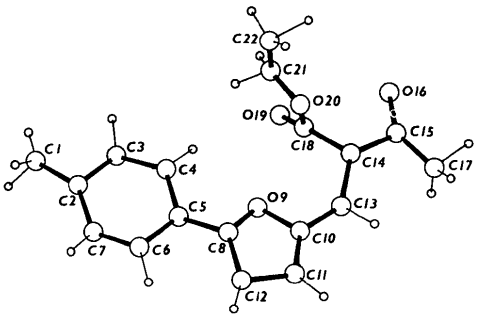

Fig. 1. A perspective view of the title compound showing the atomic numbering. H atoms are not labelled for clarity.

Related literature. In the crystal structure of the related compound, 3,5-diethoxycarbonyl-2,6-dimethyl-4-[5-(*p*-tolyl)-2-furyl]-1,4-dihydropyridine, the phenyl and furyl groups are somewhat less conjugated (dihedral angle 6·4°), obviously due to the less extensive π system (restricted to the phenyl and furyl groups alone) as compared with that in the title compound. The geometry of the ethoxycarbonyl group agrees with that observed systematically in the carboxylic ester groups (Merlino, 1971; Dunitz & Schweizer, 1982).

* Lists of structure factors, anisotropic displacement parameters, H-atom parameters and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52730 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Dihydro-2,3 (Thiényl-3)-2 5*H*-Benzothiazépine-1,5 One-4

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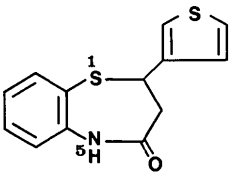
Abstract. $C_{13}H_{11}NOS_2$, $M_r = 261{\cdot}36$, monoclinic, $P2_1/n$ (second setting), $a = 7{\cdot}600$ (2), $b = 14{\cdot}581$ (6), $c = 11{\cdot}138$ (5) Å, $\beta = 93{\cdot}25$ (3)°, $V = 1232{\cdot}3$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}41$, $D_m = 1{\cdot}38$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}375$ mm^{-1}, $F(000) = 544$, room temperature, $R = 0{\cdot}046$ for 1633 independent reflections [$I > 3\sigma(I)$]. The title compound consists of a seven-membered thiazepine ring fused to a benzene ring and substituted by a 3-thienyl ring. As expected, the 1,5-benzothiazepine ring is not planar; the dihedral angle between the benzene and thienyl rings is 46·5 (1)°. The molecules are linked together by N(5)—H(N5)···O($-x$,1 $-$ y,2 $-$ z) hydrogen bonds [2·862 (4) Å; 172 (4)°].

Partie expérimentale. Masse volumique par flottaison. Cristal prismatique, 0,22 × 0,30 × 0,38 mm. Dimensions de la maille déterminées sur monocristal à partir de 25 réflexions telles que $3{,}08 \le \theta \le 171{,}71°$. Diffractomètre Syntex–Nicolet *P*3*F* ($2\theta \le 60°$); $-12 \le h \le 12$; $0 \le k \le 22$; $0 \le l \le 16$. Réflexions de contrôle $\bar{3}\bar{1}0$, $\bar{1}30$; $\sigma(I)/I$ contrôle = 0,02. 3740 réflexions indépendantes mesurées, 1633 observées [$I > 3\sigma(I)$]. Pas de correction d'absorption. Méthodes directes, programme *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Coordonnées des H: série de Fourier des ΔF. Facteurs de diffusion des *International Tables for X-ray Crystallography* (1974). Affinement sur F. Paramètres affinés: x,y,z de tous les atomes et U_{ij} de O, N, C et S. $R = 0{,}046$; $wR = 0{,}050$, $w = 1/\sigma(F)$, $S = 1{,}9$. $(\Delta/\sigma)_{max} = 1{,}6$ [valeur observée pour H(32)].



$(\Delta/\sigma)_{moyen} = 0{,}11$; $|\Delta\rho|_{max} = 0{,}24$ e Å^{-3}. Programme de calcul *ORXFLS* de Busing (1971). Calcul des angles dièdres, programme *BP*7*C* (Ito & Sugawara, 1983). Dessin de la molécule (Fig. 1) et vue stéréoscopique du contenu de la maille (Fig. 2), programme *ORTEP*II (Johnson, 1976).

Les paramètres atomiques sont rassemblés dans le Tableau 1, les distances et les angles dans le Tableau

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