Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(*N*-Ethylthiocarbamoyl)-3,5-di-2-furyl-2-pyrazoline

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.139
Data-to-parameter ratio = 14.5

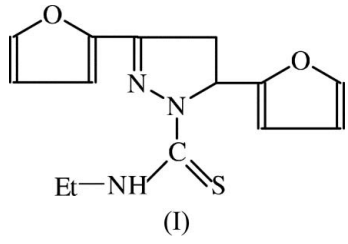
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 7 June 2005
Accepted 16 June 2005
Online 24 June 2005

The molecule of the title compound, $C_{14}H_{15}N_3O_2S$, is non-planar; the dihedral angle between the two furyl rings is 88.4 (2)°. The crystal structure is stabilized by one C—H···π interaction.

Comment

Pyrazoles are widely studied five-membered heterocyclic compounds and their syntheses have been extensively studied (Parmar *et al.*, 1974; Soni *et al.*, 1987). These studies have been stimulated by some promising pharmacological, agrochemical and analytical applications (Polevoi, 1966; Batulin, 1969; Palaska *et al.*, 1996). Compounds including a pyrazole nucleus are known to posses analgesic, anti-inflammatory, antipyretic, antiarrhythmic, tranquillizing, muscle relaxant, psycho-analeptic, anticonvulsant, hypotensive, monoamine oxidase inhibitor, antidiabetic and antibacterial activities (Bruno *et al.*, 1993; Mazzone *et al.*, 1986).



(I)

The molecule of the title compound, (I), is non-planar, the dihedral angles between furyl rings O1/C1–C4 and O2/C8–C11 and the pyrazoline ring being 6.3 (2) and 85.59 (18)°, respectively. The dihedral angle between the two furyl rings is 88.4 (2)°. The crystal structure is stabilized by one C—H···π interaction (Table 1).

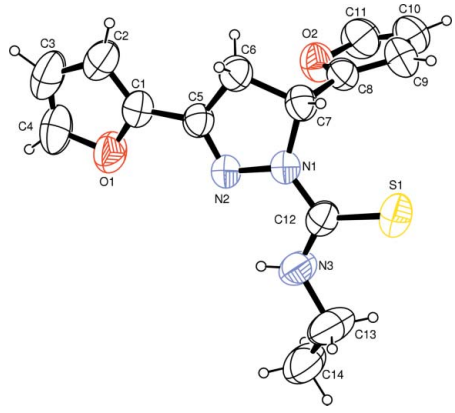


Figure 1
An *ORTEP-3* view (Farrugia, 1997) of the title compound, showing the atom-numbering scheme and 50% probability displacement ellipsoids.

Experimental

1,3-Di-2-furyl-2-propen-1-one (0.01 mol) was dissolved in ethanol (25 ml). Hydrazine hydrate (1 g, 0.02 mol) was then added. The solution was warmed in a water bath for 2 h. After cooling, the solvent was entirely removed under reduced pressure and 3,5-di-2-furyl-2-pyrazoline was obtained. The compound was dissolved in dry diethyl ether (25 ml) and then ethyl isothiocyanate (0.01 mol) and four drops of triethylamine were added. The solution was stirred for 4 h at room temperature. After removing the solvent, the residue was recrystallized from ethanol to give the compound (I) (yield 47%; m.p. 406–408 K).

Crystal data

$C_{14}H_{15}N_3O_2S$
M_r = 289.35
Monoclinic, $P2_1/c$
a = 7.0192 (4) Å
b = 22.1771 (10) Å
c = 10.5972 (7) Å
β = 119.541 (4)°
V = 1435.17 (14) Å^3
Z = 4
D_x = 1.330 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9837 reflections
θ = 1.8–27.2°
μ = 0.23 mm^{-1}
T = 293 (2) K
Prism, yellow
0.56 × 0.50 × 0.43 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.879, T_{max} = 0.879
13798 measured reflections
2808 independent reflections
2420 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 26.0°
$h = -8 \rightarrow 8$
$k = -24 \rightarrow 27$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.139
S = 1.06
2808 reflections
193 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1115P)^2 + 0.5302P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

Cg is the centroid of the furyl O2/C8–C11 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cg^i	0.93	2.86	3.763 (3)	165

Symmetry code: (i) $x + 1, y, z$.

All H atoms, except for H6*A*, H6*B* and H7, were treated using a riding model, with C—H = 0.93 (aromatic H), 0.97 (methylene H) or 0.96 Å (methyl H). The U_{iso}(H) values were constrained to be 1.2 (1.5 for the methyl group) times U_{eq}(C). Atoms H6*A*, H6*B* and H7 were refined isotropically.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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