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Ethyl 4-(2,5-dioxo-2,5-dihydro-1*H*-pyrrol-1-yl)benzoate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.138
Data-to-parameter ratio = 11.2

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

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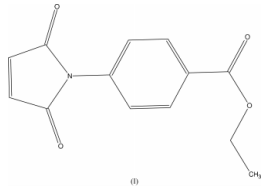
In the title compound, $C_{13}H_{11}NO_4$, the dihedral angle between the benzene and maleimide rings is 41.4 (1)°. There are C—H···O hydrogen-bonded chains, running along the *a* and *c* axes.

Comment

Succinimides are important medicinal agents in the therapy of diseases such as tuberculosis, convulsions and hypertension (Pandey *et al.*, 1984; Crider & Edward, 1977). The title compound, (I), is such a derivative with an ester-substituted aryl maleimide.



The bond lengths and bond angles are comparable with values reported for similar compounds (Rodriguez *et al.*, 2002). The angle between the mean planes passing through the benzene ring (C5–C10) and the maleimide ring (N1/C1–C4) is 41.4 (1)°, indicating the steric repulsion between the carbonyl groups and the benzene ring. The dihedral angle is small [2.5 (2) Å] in a similar structure without carbonyl groups (Paulus & Rivo, 1988).

Molecular chains are observed, *via* two different C—H···O hydrogen bonds running along the *a* and *c* axes, respectively (Table 1 and Fig. 2). The C—H···O hydrogen-bonded chain down the *a* axis involves the ester carbonyl group, whereas the

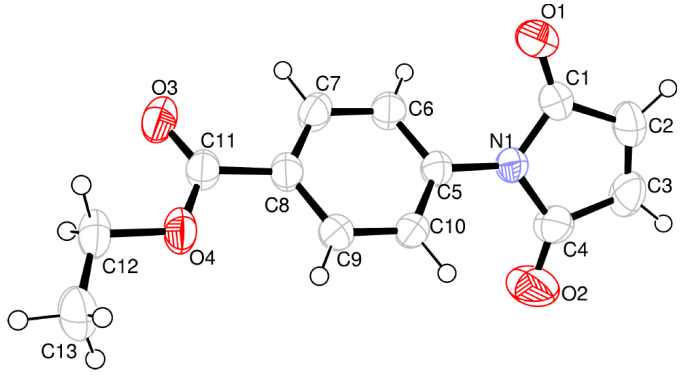


Figure 1
ORTEP-3 (Farrugia, 1997) diagram of (I), with 50% probability displacement ellipsoids.

other down the *c* axis employs one of the carbonyl groups of the maleimide ring.

Experimental

Maleanilic acid was synthesized by refluxing maleic anhydride (3.9 g, 0.04 mol), 5.5 ml of *p*-nitroaniline and 75 ml of ether. To the resulting solution, acetic anhydride (15.3 ml, 0.15 mol) and anhydrous sodium acetate (2.0 g) were added and the mixture was heated in a steam bath for 30 min. The reaction mixture was cooled to room temperature and then poured into 15 ml of ice water. The precipitated product was separated, washed with ice-cold water and aqueous sodium bicarbonate and dried. Light yellow crystals of (I) were obtained by slow evaporation of a methanol solution.

Crystal data

$C_{13}H_{11}NO_4$	D_x = 1.365 Mg m^{-3}
M_r = 245.23	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 775 reflections
a = 12.028 (6) Å	θ = 2.2–25.5°
b = 7.358 (4) Å	μ = 0.10 mm^{-1}
c = 13.561 (7) Å	T = 293 (2) K
β = 96.364 (7)°	Prism, pale yellow
V = 1192.9 (11) Å^3	0.40 × 0.30 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2328 independent reflections
φ and ω scans	1965 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.013
T_{min} = 0.903, T_{max} = 0.980	θ_{max} = 26.4°
8371 measured reflections	$h = -14 \rightarrow 15$
	$k = -9 \rightarrow 9$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0933P)^2 + 0.1715P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.138	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
S = 1.00	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
2328 reflections	
207 parameters	
All H-atom parameters refined	

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O3^{i}	0.94 (2)	2.51 (2)	3.402 (3)	158 (2)
C10—H10···O1^{ii}	0.98 (2)	2.61 (2)	3.426 (3)	141 (1)

Symmetry codes: (i) $1+x, y, z$; (ii) $x, \frac{1}{2}-y, \frac{1}{2}+z$.

The H atoms were refined isotropically. The C—H bond lengths are 0.92 (2)–0.99 (2) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 1990).

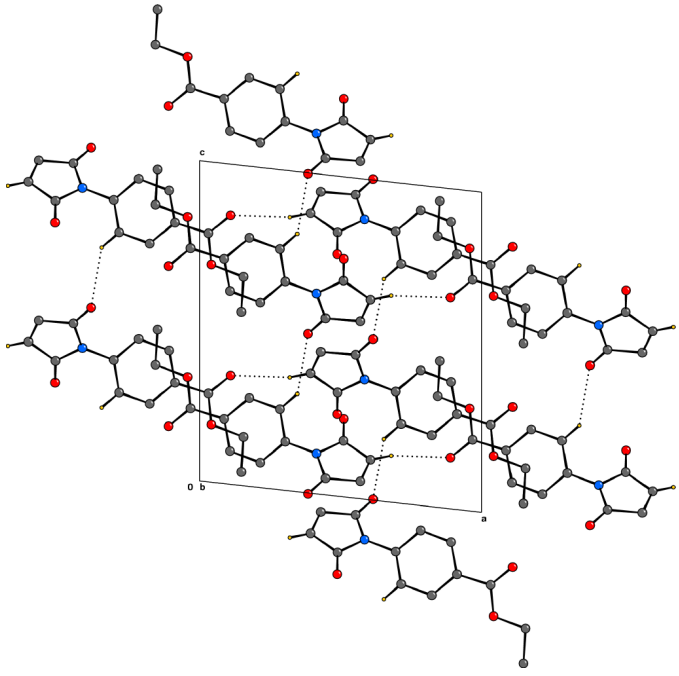


Figure 2
Packing diagram of (I), viewed down the *b* axis. The dotted lines represent C—H···O hydrogen bonds.

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