

# 4'-{[2-(But-2-enyl)-4-chloro-5-formyl-1*H*-imidazol-1-yl]methyl}biphenyl-2-carbonitrile

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## Key indicators

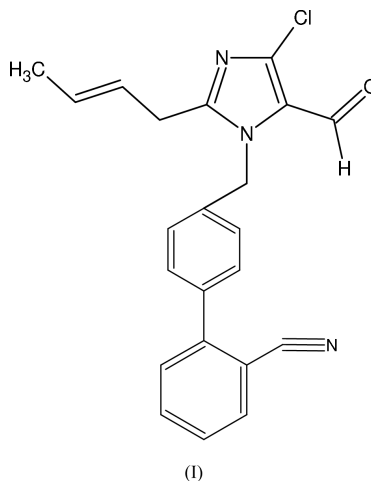
Single-crystal X-ray study  
 $T = 293\text{ K}$   
 Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.064  
 $wR$  factor = 0.184  
 Data-to-parameter ratio = 17.0

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

In the title structure,  $\text{C}_{22}\text{H}_{18}\text{ClN}_3\text{O}$ , the dihedral angle between the benzene rings of the biphenyl system is  $41.6(1)^\circ$ ; they are approximately perpendicular to the planar imidazole ring. The crystal structure is stabilized by  $\text{C}-\text{H}\cdots\text{Cl}$ ,  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds and  $\text{C}-\text{H}\cdots\pi$  interactions.

## Comment

Imidazole is a fundamental building block of many proteins and other biological systems. It also acts as a ligand that will bind readily to a metal ion in aqueous systems. Imidazole-4-acetic acid is a catabolite of histamine and is present in the brain (Prell *et al.*, 1996), and an imidazole succinic acid complex is an active non-steroidal aromatase inhibitor (Schiavo *et al.*, 1988). The title compound, (I), serves as a key intermediate for the preparation of the antihypertensive drug losartan potassium (Griffiths *et al.*, 1999).



As expected, the cyanide group is linear, with angle  $\text{C14}-\text{C19}-\text{N20}$  equal to  $176.9(3)^\circ$ . Angles  $\text{C9}-\text{C10}-\text{C11}$  of  $117.6(2)^\circ$  and  $\text{C14}-\text{C13}-\text{C18}$  of  $117.1(2)^\circ$  are contracted, due to the steric hindrance of the biphenyl system. The but-2-enyl chain is in an extended conformation, as noted from the torsion angles  $\text{N1}-\text{C2}-\text{C21}-\text{C22}$  [ $156.2(3)^\circ$ ],  $\text{C2}-\text{C21}-\text{C22}-\text{C23}$  [ $-165.5(5)^\circ$ ] and  $\text{C21}-\text{C22}-\text{C23}-\text{C24}$  [ $178.0(5)^\circ$ ]. The dihedral angle between the benzene rings of the biphenyl system is  $41.6(1)^\circ$ ; rings  $\text{C7}-\text{C12}$  and  $\text{C13}-\text{C18}$  make angles of  $73.3(1)^\circ$  and  $85.9(1)^\circ$ , respectively, with the plane of the imidazole ring.

The crystal structure of (I) is stabilized by  $\text{C}-\text{H}\cdots\text{Cl}$ ,  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds and  $\text{C}-\text{H}\cdots\pi$  interactions (Table 1 and Fig. 2). The two interactions  $\text{C}-\text{H}\cdots\text{Cl}$  and the  $\text{C}-\text{H}\cdots\text{N}$  involving atom N3 of the imidazole result

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in the formation of a two-dimensional network in the *bc* plane. A C—H... $\pi$  interaction exists between C11 and benzene ring C13–C18 at  $(-x, -y, 1 - z)$ , the distance between C11 and the centroid of the ring being 3.983 Å.

## Experimental

To a suspension of sodium methoxide (0.03 mol, 1.62 g) in dimethylformamide (DMF, 25 ml) was added a solution of 2-(but-2-enyl)-4-chloro-5-formylimidazole (0.03 mol, 5.655 g) in DMF. The mixture was stirred at 298 K for 30 min, and to this was added dropwise a solution of 4-bromomethyl-2'-cyanobiphenyl (0.025 mol, 6.80 g) in DMF (25 ml). The mixture was stirred at room temperature for 24 h and evaporated to a residue under vacuum. The residue was dissolved in ethyl acetate (70 ml), washed with brine (20 ml), then water (50 ml), dried using Na<sub>2</sub>SO<sub>4</sub> and evaporated to yield a crude product; this was purified by column chromatography using a mixture (7:2) of *n*-hexane and ethyl acetate as eluant to give the title product, which was recrystallized from CCl<sub>4</sub>.

### Crystal data

C <sub>22</sub> H <sub>18</sub> ClN <sub>3</sub> O	$D_x = 1.273 \text{ Mg m}^{-3}$
$M_r = 375.84$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 20332 reflections
$a = 9.080$ (6) Å	$\theta = 1.8\text{--}27.4^\circ$
$b = 22.782$ (15) Å	$\mu = 0.21 \text{ mm}^{-1}$
$c = 10.055$ (7) Å	$T = 293$ (2) K
$\beta = 109.476$ (10)°	Rectangular block, colourless
$V = 1961$ (2) Å <sup>3</sup>	$0.30 \times 0.25 \times 0.22 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART CCD area-detector diffractometer	3164 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.022$
Absorption correction: none	$\theta_{\text{max}} = 27.4^\circ$
20332 measured reflections	$h = -11 \rightarrow 11$
4143 independent reflections	$k = -29 \rightarrow 28$
	$l = -12 \rightarrow 12$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0786P)^2 + 1.127P]$
$R[F^2 > 2\sigma(F^2)] = 0.064$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.184$	$(\Delta/\sigma)_{\text{max}} = 0.083$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.64 \text{ e Å}^{-3}$
4143 reflections	$\Delta\rho_{\text{min}} = -0.36 \text{ e Å}^{-3}$
244 parameters	
H-atom parameters constrained	

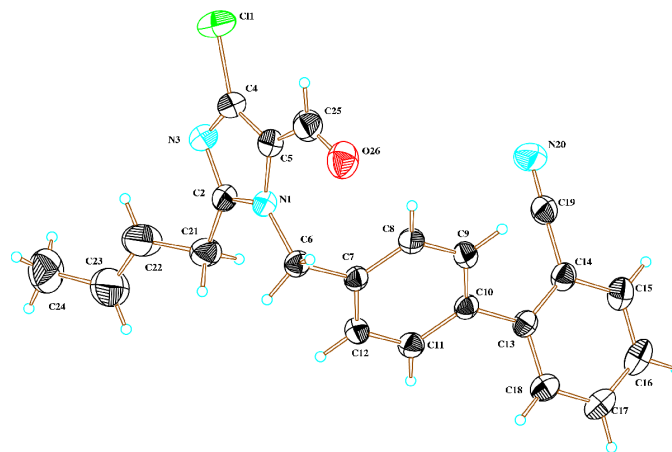
**Table 1**

Hydrogen-bonding geometry (Å, °) for (I).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
C6—H6B...O26	0.97	2.40	3.048 (3)	124
C8—H8...O26	0.93	2.71	3.463 (4)	139
C21—H21A...N20 <sup>i</sup>	0.97	2.62	3.578 (5)	170
C6—H6A...N20 <sup>j</sup>	0.97	2.68	3.625 (4)	165
C15—H15...O26 <sup>ii</sup>	0.93	2.84	3.421 (4)	122
C17—H17...N3 <sup>iii</sup>	0.93	2.74	3.532 (4)	144
C18—H18...O26 <sup>iv</sup>	0.93	2.76	3.677 (5)	171
C24—H24A...Cl <sup>v</sup>	0.96	2.91	3.818 (5)	159
C11—H11...C <sub>g</sub> <sup>vi</sup>	0.93	3.27	3.983	135

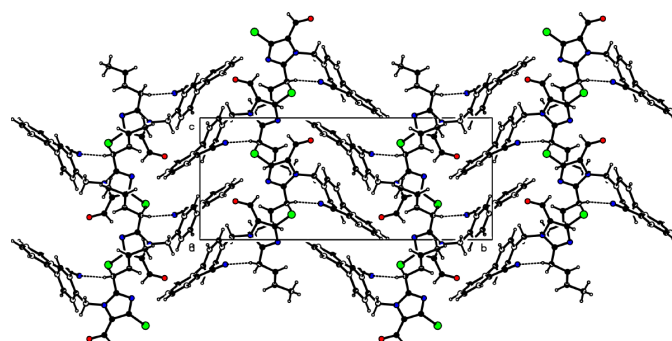
Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $1 - x, -y, -z$ ; (iii)  $-x, y - \frac{1}{2}, -\frac{1}{2} - z$ ; (iv)  $-x, -y, -z$ ; (v)  $x - 1, y, z - 1$ ; (vi)  $-x, -y, 1 - z$ . C<sub>g</sub> is the centroid of the benzene ring C13–C18.

All H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2$  or 1.5 times  $U_{\text{eq}}(\text{parent atom})$ .



**Figure 1**

ZORTEP (Zsolnai, 1998) plot of the title molecule, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.



**Figure 2**

A packing diagram of the crystal structure, viewed down the *a* axis. Dashed lines represent hydrogen bonds.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003), *ORTEP-3* (Farrugia, 1997) and *ZORTEP* (Zsolnai, 1998); software used to prepare material for publication: *PLATON*.

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