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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 K
Mean σ(C–C) = 0.004 Å
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.

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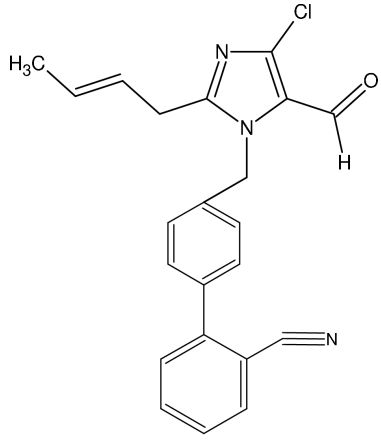
In the title structure, $C_{22}H_{18}ClN_3O$, the dihedral angle between the benzene rings of the biphenyl system is 41.6 (1)°; they are approximately perpendicular to the planar imidazole ring. The crystal structure is stabilized by C—H···Cl, C—H···O and C—H···N hydrogen bonds and C—H···π interactions.

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).



(I)

As expected, the cyanide group is linear, with angle C14—C19—N20 equal to 176.9 (3)°. Angles C9—C10—C11 of 117.6 (2)° and C14—C13—C18 of 117.1 (2)° 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 N1—C2—C21—C22 [156.2 (3)°], C2—C21—C22—C23 [−165.5 (5)°] and C21—C22—C23—C24 [178.0 (5)°]. The dihedral angle between the benzene rings of the biphenyl system is 41.6 (1)°; rings C7—C12 and C13—C18 make angles of 73.3 (1) and 85.9 (1)°, respectively, with the plane of the imidazole ring.

The crystal structure of (I) is stabilized by C—H···Cl, C—H···O and C—H···N hydrogen bonds and C—H···π interactions (Table 1 and Fig. 2). The two interactions C—H···Cl and the C—H···N involving atom N3 of the imidazole result

in the formation of a two-dimensional network in the *bc* plane. A C—H···π 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_2SO_4 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_4.

Crystal data

$C_{22}H_{18}ClN_3O$
M_r = 375.84
Monoclinic, $P2_1/c$
a = 9.080 (6) Å
b = 22.782 (15) Å
c = 10.055 (7) Å
β = 109.476 (10)°
V = 1961 (2) Å^3
Z = 4
D_x = 1.273 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20332 reflections
θ = 1.8–27.4°
μ = 0.21 mm^{-1}
T = 293 (2) K
Rectangular block, colourless
0.30 × 0.25 × 0.22 mm

Data collection

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

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···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^{i}	0.97	2.62	3.578 (5)	170
C6—H6A···N20^{i}	0.97	2.68	3.625 (4)	165
C15—H15···O26^{ii}	0.93	2.84	3.421 (4)	122
C17—H17···N3^{iii}	0.93	2.74	3.532 (4)	144
C18—H18···O26^{iv}	0.93	2.76	3.677 (5)	171
C24—H24A···Cl1^{v}	0.96	2.91	3.818 (5)	159
C11—H11···Cg^{vi}	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) $-x, -y, 1 - z$. Cg 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_{iso}(H) = 1.2 or 1.5 times U_{eq}(parent atom).

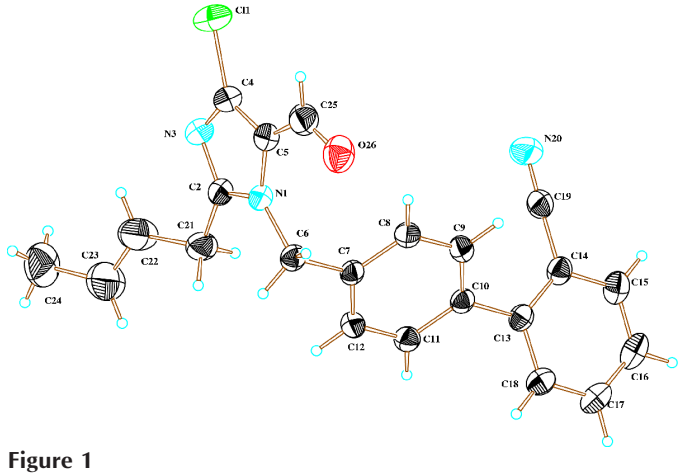


Figure 1
ZORTEP (Zsolnai, 1998) plot of the title molecule, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

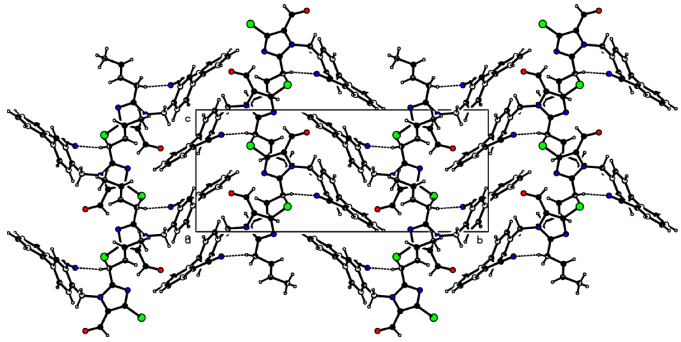


Figure 2
A packing diagram of the crystal structure, viewed down the *a* axis. Dashed lines represent hydrogen bonds.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (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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