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Methyl 4-[(2-butyl-4-chloro-5-formyl-1*H*-imidazol-1-yl)methyl]benzoate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.059
wR factor = 0.178
Data-to-parameter ratio = 14.7

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

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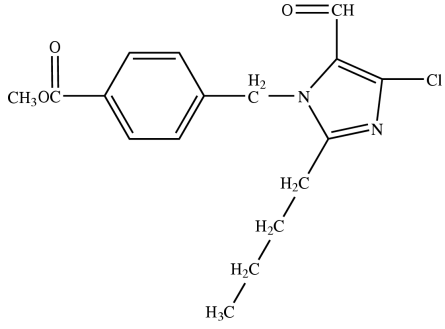
In the title compound, $C_{17}H_{19}ClN_2O_3$, the dihedral angles formed by the butyl group and the imidazole ring with the benzene ring are 86.4 (4) and 88.9 (3)°, respectively. The dihedral angle between the imidazole ring and the butyl group is 77.1 (5)°. The structure is stabilized by C—H···O and C—H···π interactions.

Comment

The renin–angiotensin system (RAS) plays an important role in the regulation of blood pressure and fluid and electrolyte balance. Blockage of the renin–angiotensin system by inhibiting the biosynthesis of the effector hormone, angiotensin II (AII), with angiotensin-converting enzyme (ACE) inhibitors has been shown to be clinically effective in the treatment of hypertension, congestive heart failure and, potentially, chronic renal failure (Corvol, 1989). However, ACE inhibitors, in addition to their effects on the RAS, inhibit bradykinin metabolism, and as a result may produce coughs and angioedema. An alternative, and perhaps more selective, approach to interfering with the RAS is to inhibit the binding of AII to its receptor. Although a number of peptide analogs of AII have been reported to have AII receptor antagonist properties, all have retained partial agonist properties and have lacked oral bioavailability. More recently, several groups have described non-peptide AII receptor antagonists that show promise as inhibitors of the RAS (Dunica *et al.*, 1990). We describe here the structure of the title compound, (I), a highly potent selective non-peptide AII receptor antagonist which was designed to mimic the C-terminal region of AII.



(I)

In the title compound, bond lengths and angles in the benzene and imidazole rings are comparable with those reported in the literature (Ji *et al.*, 2002; Jian *et al.*, 2002). The C—Cl bond length [1.717 (4) Å] is shorter than others reported [1.773 (8) (Pretsch *et al.*, 2000) and 1.742 (3) Å (Liu *et al.*, 1999)]. The C atoms of the butyl chain are in a plane (*P*1). The imidazole ring is approximately planar with its

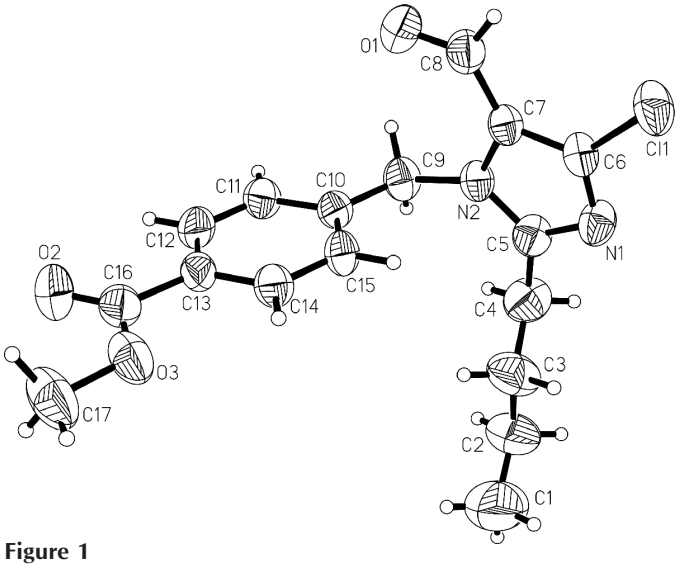


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

immediate substituent atoms Cl1, C8, O1 and C9 (*P*2), with a maximum deviation of 0.050 (1) Å for C9. The benzene ring is planar with its immediate substituent atoms C9, C16, C17, O2 and O3 (*P*3), with the largest deviation of 0.052 (1) Å for O2. The dihedral angles formed by *P*1 and *P*2 with *P*3 are 86.4 (4) and 88.9 (3)°, respectively. The dihedral angle between *P*1 and *P*2 is 77.1 (5)°.

The molecular structure is stabilized by intramolecular C—H···π interactions [C9···*Cg*2 = 3.675 Å, H9*A*···*Cg*2 = 3.34 Å, H9*B*···*Cg*2 = 3.34 Å, C9—H9*A*···*Cg*2 = 103° and C9—H9*B*···*Cg*2 = 103° (symmetry code: $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$); C12···*Cg*1 = 3.570 Å, H12*A*···*Cg*1 = 3.27 Å and C12—H12*A*···*Cg*1 = 101° (symmetry code: $\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$); C17···*Cg*2 = 3.535 Å, H17*B*···*Cg*2 = 2.79 Å and C17—H17*B*···*Cg*2 = 135° (symmetry code: $1-x, -y, -z$); *Cg*1 is the imidazole ring centroid and *Cg*2 is the benzene ring centroid]. In addition, there are two C—H···O interactions (Table 1), one intermolecular and the other intramolecular, involving the same atoms.

Experimental

The title compound was prepared by the reaction of 2-butyl-4-chloro-1*H*-imidazole-5-carboxaldehyde (30.4 g, 200 mmol) with methyl 4-(bromomethyl)benzoate (50.5 g, 220 mmol) in dimethylformamide (90 ml) at 273 K. Single crystals suitable for X-ray measurements were obtained by recrystallization from dimethylformamide at room temperature.

Crystal data

$C_{17}H_{19}ClN_2O_3$
M_r = 334.79
Monoclinic, $P2_1/n$
a = 11.946 (2) Å
b = 9.7085 (19) Å
c = 15.247 (3) Å
β = 99.26 (3)°
V = 1745.2 (6) Å^3
Z = 4
D_x = 1.274 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 4–14°
μ = 0.23 mm^{-1}
T = 293 (2) K
Prism, colorless
0.30 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
3226 measured reflections
3070 independent reflections
1705 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.1°
$h = -14 \rightarrow 0$
$k = -11 \rightarrow 0$
$l = -17 \rightarrow 18$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.178
S = 1.04
3070 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 1.4956P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0047 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9*A*···O1^{i}	0.97	2.55	3.491 (5)	165
C9—H9*B*···O1	0.97	2.49	2.998 (5)	112

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

The H atoms were positioned geometrically and treated as riding on the parent C atoms, with C—H distances in the range 0.93–0.97 Å and $U_{iso} = 1.2U_{eq}$(C).

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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