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Iodometronidazole

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.039
wR factor = 0.104
Data-to-parameter ratio = 14.1

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

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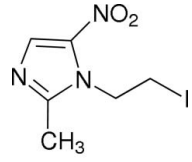
In the title compound, 1-(2-iodoethyl)-2-methyl-5-nitro-1*H*-imidazole, $C_6H_8IN_3O_2$, the dihedral angle between the imidazole ring and the nitro group attached to it is 7.8 (1)°.

Comment

The molecular structure of the title compound, (I), is shown in Fig. 1. It is quite similar to chlorometronidazole. The imidazole ring in each molecule is planar, with an average deviation of 0.009 (1) Å. The nitro N atom is 0.017 (1) Å above the plane; the other two groups attached to the ring are located on the opposite side of the plane, with displacements of 0.229 (1) (for C5) and 0.027 (1) Å (for C4) from the plane of the ring. The dihedral angle between the imidazole ring and the nitro plane is 7.8 (1)°.



(I)

Experimental

To a pyridine solution (5 ml) of chlorometronidazole (190 mg, 1 mmol) was added NaI (165 mg, 1.1 mmol). This mixture was stirred for 5 h at 313 K. The solvents were removed and the residue recrystallized from chloroform. Large crystals suitable for X-ray crystal structure determination formed in 2 d. These were collected by filtration, washed with chloroform and diethyl ether, and dried in a vacuum desiccator using $CaCl_2$ (yield: 91%). Elemental analysis found: C 25.7, H 2.8, N 15.0%; calculated for $C_6H_8IN_3O_2$: C 25.6, H 2.9, N 14.9%. Chlorometronidazole was prepared as described in the preceding paper (Pi *et al.*, 2005).

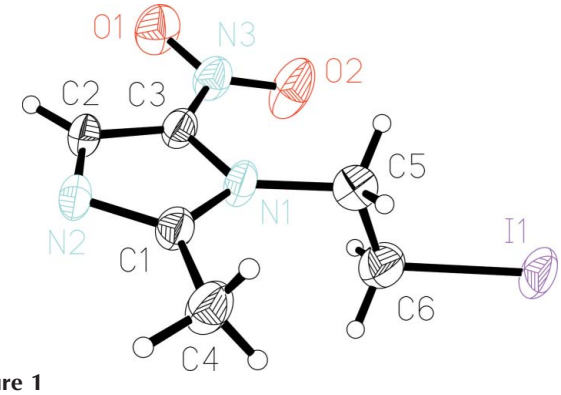


Figure 1
The molecular structure of the title compound, (I), showing 30% probability displacement ellipsoids for the non-H atoms and the atom-numbering scheme.

Crystal data

$C_6H_8IN_3O_2$	$Z = 2$
$M_r = 281.05$	$D_x = 2.039$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 6.192$ (3) Å	Cell parameters from 1310 reflections
$b = 7.740$ (3) Å	$\theta = 6.1$–$25.8°$
$c = 10.001$ (4) Å	$\mu = 3.46$ mm^{-1}
$\alpha = 89.073$ (6)°	$T = 298$ (2) K
$\beta = 86.903$ (6)°	Prism, pale yellow
$\gamma = 73.097$ (6)°	0.40 × 0.35 × 0.35 mm
$V = 457.9$ (3) Å^3	

Data collection

Siemens SMART CCD area-detector diffractometer	1553 independent reflections
φ and ω scans	1410 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.011$
$T_{min} = 0.265$, $T_{max} = 0.298$	$\theta_{max} = 25.0°$
2006 measured reflections	$h = -7 \rightarrow 7$
	$k = -7 \rightarrow 9$
	$l = -10 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 1.1805P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.039$	$(\Delta/\sigma)_{max} = 0.004$
$wR(F^2) = 0.104$	$\Delta\rho_{max} = 0.94$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.88$ e Å^{-3}
1553 reflections	
110 parameters	
H-atom parameters constrained	

All H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.96 Å. They were treated as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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