4-Ethyl-5-(N-hydroxy-N-phenylamino)-2-phenyl-3-propylisoxazolidine

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Abstract. $C_{20}H_{26}N_2O_2$, $M_r = 326.4$, monoclinic, $P2_1/n$, $a = 12.350$ (2), $b = 6.7807$ (9), $c = 22.006$ (4) Å, $\beta = 99.68$ (1)°, $V = 1816.6$ Å^3, $Z = 4$, $D_x = 1.19$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 0.043$ mm^{-1}, $F(000) = 704$, $T = 293$ K, $R = 0.050$ for 1767 unique reflexions $[F > 3\sigma(F)]$. The isoxazolidine ring has assumed a half-chair conformation with all substitutents in axial positions. Intermolecular hydrogen bonds between the hydroxyl H and the ring O link the molecules into centrosymmetric dimers $[\text{O} \cdots \text{O } 2.760$ (5), $\text{H} \cdots \text{O } 1.95$ (5) Å$]$.

Experimental. The title compound was synthesized by the method of Utzinger & Regenass (1954). Crystal dimensions $0.3 \times 0.3 \times 0.3$ mm, Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$ radiation, unit-cell dimensions from setting angles of 25 accurately centred reflexions $(7.3 < \theta < 11.5°)$, ω–2θ-scan mode used to measure 2571 reflexions with $I > 0$, ω-scan speed ranging from 0.9 to 5° min^{-1}

Table 1. *Fractional atomic coordinates* $(\times 10^4)$ *and vibrational parameters* ($\text{Å}^2 \times 10^4$) *for non-H atoms*

	x	y	z	U_{eq}*
N(1)	7561 (2)	4266 (3)	392 (1)	452
C(2)	7284 (3)	2218 (4)	546 (1)	458
C(3)	6676 (2)	2426 (4)	1091 (1)	442
C(4)	6263 (2)	4561 (4)	1044 (1)	411
O(5)	6617 (1)	5365 (3)	496 (1)	456
C(6)	8550 (2)	5097 (4)	729 (1)	438
C(7)	8567 (3)	6845 (5)	1046 (1)	526
C(8)	9551 (3)	7613 (5)	1347 (2)	628
C(9)	10525 (3)	6673 (6)	1329 (2)	655
C(10)	10513 (3)	4957 (5)	1001 (2)	698
C(11)	9540 (3)	4169 (5)	700 (2)	618
C(12)	6611 (3)	1225 (5)	−17 (1)	563
C(13)	7199 (4)	1017 (6)	−564 (2)	701
C(14)	8124 (4)	−449 (8)	−473 (2)	860
C(15)	7398 (3)	2018 (6)	1716 (1)	576
C(16)	6789 (4)	2143 (6)	2255 (2)	667
N(17)	5097 (2)	4950 (3)	964 (1)	462
O(18)	4504 (2)	3372 (3)	628 (1)	595
C(19)	4666 (2)	5386 (5)	1509 (1)	464
C(20)	3875 (3)	4272 (6)	1713 (2)	698
C(21)	3493 (3)	4806 (8)	2246 (2)	852
C(22)	3890 (3)	6408 (7)	2576 (2)	802
C(23)	4665 (3)	7546 (7)	2369 (2)	749
C(24)	5045 (3)	7066 (5)	1836 (2)	620

$$* U_{eq} = \tfrac{1}{3}\textstyle\sum_i \sum_j U_{ij} \mathbf{a}_i \cdot \mathbf{a}_j a_i^* a_j^*.$$

Table 2. *Selected bond lengths* (Å)

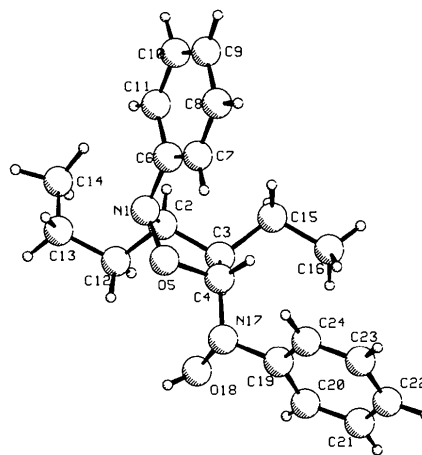|			
N(1)–C(2)	1.483 (3)	N(1)–O(5)	1.434 (3)
N(1)–C(6)	1.434 (3)	C(2)–C(3)	1.525 (4)
C(2)–C(12)	1.526 (4)	C(3)–C(4)	1.532 (4)
C(3)–C(15)	1.533 (4)	C(4)–O(5)	1.457 (3)
C(4)–N(17)	1.445 (3)	C(6)–C(7)	1.374 (4)
C(6)–C(11)	1.385 (4)	C(7)–C(8)	1.384 (4)
C(8)–C(9)	1.368 (4)	C(9)–C(10)	1.368 (5)
C(10)–C(11)	1.379 (4)	C(12)–C(13)	1.514 (5)
C(13)–C(14)	1.502 (5)	C(15)–C(16)	1.511 (5)
N(17)–O(18)	1.430 (3)	N(17)–C(19)	1.422 (3)
C(19)–C(20)	1.369 (4)	C(19)–C(24)	1.387 (4)
C(20)–C(21)	1.385 (5)	C(21)–C(22)	1.353 (5)
C(22)–C(23)	1.365 (5)	C(23)–C(24)	1.374 (5)

Fig. 1. *PLUTO* (Motherwell & Clegg, 1978) drawing of the title compound showing atom labelling.

according to the intensity gathered in a pre-scan, $0 \le h \le 14$, $0 \le k \le 8$, $-26 \le l \le 26$, $0 < \theta < 25°$, 1767 unique structure amplitudes with $F > 3\sigma(F)$, $R_{int} = 0.013$, negligible drift in three intensity standards $(420, 50\bar{1}, 3\bar{1}9)$ measured every 2.5 h, Lorentz and polarization corrections but absorption ignored, *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) used to solve the phase problem, all non-H atoms found in a Fourier map, H atoms from difference Fourier map, full-matrix least squares based on F using *SHELX*76 (Sheldrick, 1976), final $R = 0.050$ [$wR = 0.040$, $w = 1.8652/\sigma^2(F_o) +$

$0 \cdot 0002 F_o^2$], anisotropic thermal parameters for heavier atoms, isotropic for H. Maximum fluctuation in final difference map in range $-0 \cdot 20$ to $+0 \cdot 19$ e Å^{-3}, maximum shift to e.s.d. ratio on final LS cycle $0 \cdot 013$ [U_{11}, C(24)]. Scattering factors from *International Tables for X-ray Crystallography* (1974), computations carried out on the joint CDC 7600/Amdahl 470 system of the University of Manchester Regional Computing Centre. Literature survey performed using the Cambridge Structural Database *via* the *Crystal Structure Search Retrieval* (1984) interactive system.

Fractional atomic coordinates and vibrational parameters are listed in Table 1* and selected bond lengths in Table 2. The molecule, including labelling scheme, is displayed in Fig. 1.

Related literature. Physicochemical properties of the title molecule have been determined by Kliegel (1969)

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* Lists of structure factors, H-atom coordinates, anisotropic vibrational parameters and complete geometry tables have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44067 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

and structural details of a similar compound published by Foster, Iball & Nash (1974).

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