

## 2-(2,6-Diisopropylphenylimino)-1-phenylpropan-1-one

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## Key indicators

Single-crystal X-ray study  
T = 295 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
R factor = 0.048  
wR factor = 0.144  
Data-to-parameter ratio = 13.5

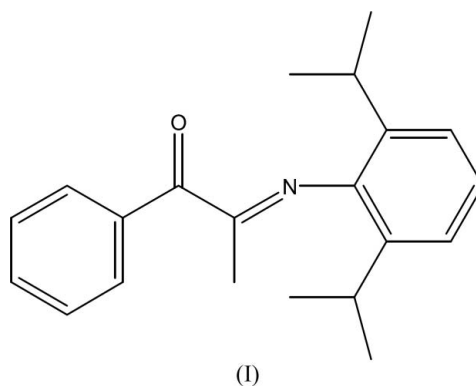
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the title compound,  $\text{C}_{20}\text{H}_{25}\text{NO}$ , all bond lengths and angles show normal values. Non-classical hydrogen bonds are responsible for the deviation from a planar arrangement.

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## Comment

In the past few years,  $\alpha$ -diimines and iminoketones have attracted interest as ligands in the synthesis of complexes used as catalysts in olefin polymerization reactions (Koten & Vrieze, 1980; Johnson *et al.*, 1995; Binotti *et al.*, 2004). Crystallographic studies of free iminoketones are relatively scarce compared to  $\alpha$ -diimines. The present communication describes the chief characteristics of 2-(2,6-diisopropylphenylimino)-1-phenylpropan-1-one, (I).



The structure of (I) can be discussed in terms of its hydrogen-bonding scheme. The individual molecules show intramolecular non-classical hydrogen bonds including a trifurcated acceptor geometry ( $\text{C6}-\text{H6}$ ,  $\text{C16}-\text{H16}$ ,  $\text{C19}-\text{H19}$ ) $\cdots\text{N1}$  (Jeffrey *et al.*, 1985), with atom N1 located 0.27 (1)  $\text{\AA}$  above the plane of the three H atoms (Fig. 1 and Table 2).

The non-classical hydrogen bonds  $\text{C19}-\text{H19}\cdots\text{N1}$  and  $\text{C16}-\text{H16}\cdots\text{N1}$  give rise to two five-membered rings sharing an edge (N1—C7 bond). The N1/C7/C8/C19/H19 ring is almost planar (r.m.s. deviation = 0.0764 $^\circ$ ), while the N1/C7/C12/C16/H16 ring shows a small deviation from planarity (r.m.s. deviation = 0.1121  $\text{\AA}$ ). An interplanar angle of 9.0 (1) $^\circ$  is observed between the rings. If we take into account the third non-classical hydrogen bond, *viz.*  $\text{C6}-\text{H6}\cdots\text{N1}$ , additional consequences can also be inferred. The first is the formation of a six-membered ring (N1/C14/C13/C1/C6/H6), with a half-boat conformation. The second feature is the O1—C13—C14—N1 torsion angle [−150.7 (2) $^\circ$ ], which is equivalent to an angle of 27.1 (1) $^\circ$  between the planes N1/C14/C15 and O1/C13/C1.

Finally, we believe that this hydrogen bond is responsible for the 68.49 (3)° deviation from coplanarity of the phenyl ring and the ring carrying the isopropyl groups.

The values found for the C—O and C—N distances (Table 1) agree well with what is expected for this bonding mode as described in the literature (*International Tables for Crystallography*, 1985, Vol. III, p. 270).

### Experimental

2,6-Diisopropylaniline (2.85 g, 3.7 mmol) was added slowly at room temperature to a methanol solution (20 ml) of 1-phenylpropane-1,2-dione (0.55 g, 3.7 mmol) in the presence of a catalytic amount of formic acid. After 6 h of magnetic stirring, the crude yellow product was isolated by filtration, washed with cold methanol (3 × 20 ml) and dried in vacuum. Yellow block-shaped crystals suitable for X-ray diffraction were obtained by recrystallization from a methanol solution (yield 0.79 g, 70%; m.p. 368 K).

#### Crystal data

C <sub>21</sub> H <sub>25</sub> NO	Z = 4
M <sub>r</sub> = 307.42	D <sub>x</sub> = 1.114 Mg m <sup>-3</sup>
Monoclinic, P2 <sub>1</sub> /n	Mo Kα radiation
a = 9.9291 (4) Å	μ = 0.07 mm <sup>-1</sup>
b = 18.5953 (6) Å	T = 295 (2) K
c = 10.4394 (4) Å	Block, yellow
β = 108.015 (2)°	0.26 × 0.24 × 0.15 mm
V = 1832.98 (12) Å <sup>3</sup>	

#### Data collection

Bruker APEX-II CCD area-detector diffractometer	3408 independent reflections
φ and ω scans	2508 reflections with I > 2σ(I)
Absorption correction: none	R <sub>int</sub> = 0.027
16097 measured reflections	θ <sub>max</sub> = 25.5°

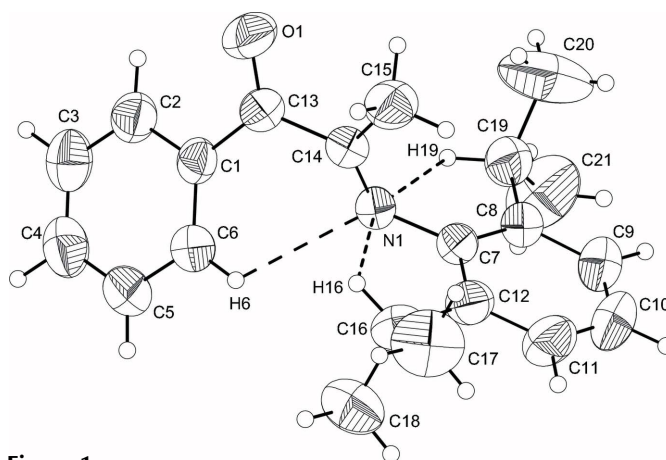
#### Refinement

Refinement on F <sup>2</sup>	w = 1/[σ <sup>2</sup> (F <sub>o</sub> <sup>2</sup> ) + (0.0598P) <sup>2</sup> + 0.2624P]
R[F <sup>2</sup> > 2σ(F <sup>2</sup> )] = 0.048	where P = (F <sub>o</sub> <sup>2</sup> + 2F <sub>c</sub> <sup>2</sup> )/3
wR(F <sup>2</sup> ) = 0.144	(Δ/σ) <sub>max</sub> = 0.001
S = 1.07	Δρ <sub>max</sub> = 0.18 e Å <sup>-3</sup>
3408 reflections	Δρ <sub>min</sub> = -0.17 e Å <sup>-3</sup>
253 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters (Å, °).

C13—O1	1.2147 (19)	C14—N1	1.2735 (19)
C13—C14	1.519 (2)		
O1—C13—C1	120.54 (14)	C15—C14—C13	116.38 (13)
O1—C13—C14	117.38 (15)	C14—N1—C7	121.32 (13)
N1—C14—C15	126.89 (14)	C14—N1—H6	91.4 (4)
N1—C14—C13	116.59 (14)	C7—N1—H6	128.0 (4)



**Figure 1**  
Perspective view of (I). Displacement ellipsoids are drawn at the 50% probability level.

**Table 2**

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C6—H6...N1	0.95 (2)	2.47 (2)	2.967 (2)	112.3 (15)
C16—H16...N1	0.96 (2)	2.56 (2)	2.943 (2)	103.9 (13)
C19—H19...N1	0.97 (2)	2.37 (2)	2.856 (2)	110.3 (14)

Phenyl and methine H atoms were located in a Fourier difference map and refined freely. Methyl H atoms were positioned geometrically, the C—H distances fixed (0.96 Å for Csp<sup>3</sup> H atoms), and the atoms refined as riding on their respective C atoms, with an isotropic displacement parameter 1.5 times U<sub>eq</sub> for the attached Csp<sup>3</sup> atom. The methyl groups were refined as rigid groups, with rotation around the respective C—C bonds as a free variable.

Data collection: *COSMO* and *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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