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O-Isobutyl *N*-phenylthiocarbamate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.117
Data-to-parameter ratio = 18.8

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

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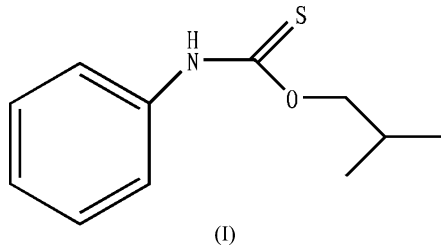
The title compound, $C_{11}H_{15}NOS$, was prepared by the reaction of phenyl isothiocyanate with isobutyl alcohol at room temperature. The central CNC(=S)O group is essentially planar. In the crystal structure, the molecules are connected *via* N—H···S interactions.

Comment

The title compound, (I), is known to coordinate metal centres in a variety of coordination modes involving all combinations of the S, O and N atoms. The compound was synthesized as part of our study of these ligands.



(I)

In the crystal structure of (I) (Fig. 1), the C—N, C—O and C—S bond lengths are similar to those found in the *O*-ethyl analogue, EtOC(S)N(H)Ph (Taylor & Tiekink, 1994), and the *O*-methyl analogue, MeOC(S)N(H)Ph (Ho *et al.*, 2003). The molecules are connected by weak N—H···S hydrogen bonds (Table 2).

Experimental

A mixture of phenyl isothiocyanate (0.1 mol) and isobutyl alcohol (0.1 mol) was stirred in 1,4-dioxane (20 ml) for 2 h at room temperature to afford the title compound (yield 75%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_{11}H_{15}NOS$
M_r = 209.30
Monoclinic, $C2/c$
a = 27.129 (5) Å
b = 6.0663 (12) Å
c = 15.613 (3) Å
β = 118.07 (3)°
V = 2267.1 (8) Å^3
Z = 8
D_x = 1.226 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 295 (2) K
Block, colourless
0.30 × 0.25 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
5077 measured reflections
2389 independent reflections
1770 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.1°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.7703P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.117$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.20$ e Å^{-3}
2389 reflections	
127 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

S1—C7	1.6700 (19)	N1—C7	1.335 (2)
O1—C7	1.322 (2)	N1—C6	1.424 (2)
O1—C8	1.452 (2)		
C7—N1—C6	131.91 (17)	O1—C7—N1	112.75 (16)
C1—C6—N1	116.14 (17)	O1—C7—S1	125.66 (14)
C5—C6—N1	124.97 (17)	N1—C7—S1	121.56 (15)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···S1^{i}	0.86	2.54	3.3971 (19)	173

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

H atoms were positioned geometrically and refined using a riding model with N—H and C—H distances of 0.86 and 0.93–0.98 Å, respectively, and with U_{iso}(H) = 1.2U_{eq}(parent atom) (1.5 for methyl groups).

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: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

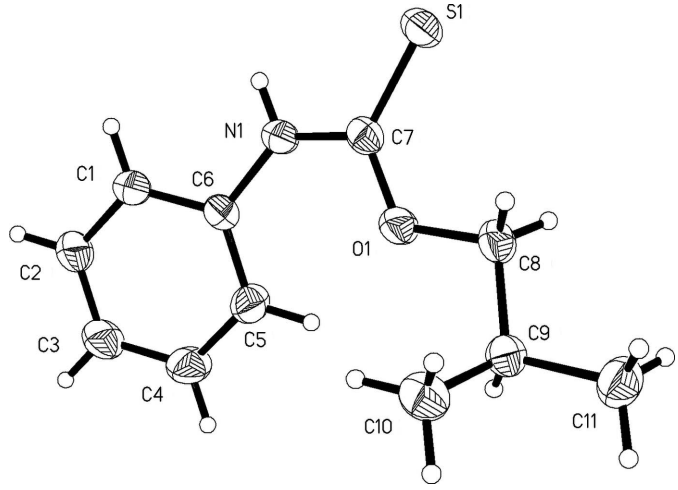


Figure 1
The molecular structure and atom-labelling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

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