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Cyclohexyl 2-(piperidin-1-ylthiocarbonylsulfanyl)-acetate

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The title compound, $C_{14}H_{23}NO_2S_2$, crystallizes with the piperidine ring in a chair conformation. Weak C—H···S hydrogen bonding helps to stabilize the crystal structure.

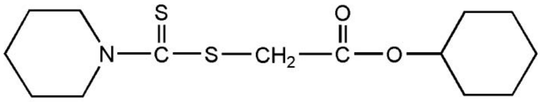
Key indicators

Single-crystal X-ray study
T = 273 K
Mean *σ*(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.096
Data-to-parameter ratio = 17.7

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

Comment

Substituted piperidines are an important class of compounds as subunits in a number of biologically active compounds (Takemoto *et al.*, 1999; Nishi *et al.*, 1998). The crystal structure of the title compound, (I), is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. The piperidine ring has a chair conformation; the average C—N and C—C bond distances [1.470 (2) and 1.509 (3) Å, respectively] within the piperidine ring are in agreement with those found in a related compound (Yuan *et al.*, 2004). The C8—O1 bond is significantly shorter than the C9—O1 bond, while the C6—N1 bond is much shorter than the C1—N1 bond. The molecules are connected by weak C—H···S hydrogen bonding (Table 1).

Experimental

Sodium piperidine-1-carbodithioate (3.66 g, 0.02 mol) and cyclohexyl 2-chloroacetate (3.52 g, 0.02 mol) were dissolved in 50 ml of ethanol. The solution was stirred for 5 h at about 273 K and then filtered. The filtrate was evaporated under reduced pressure to give (I) (yield 85%). Analysis found: C 55.6, H 7.5, N 4.6%; $C_{14}H_{23}NO_2S_2$ requires: C 55.7, H 7.6, N 4.6%. Single crystals of (I) were obtained by recrystallization from an ethanol solution at room temperature.

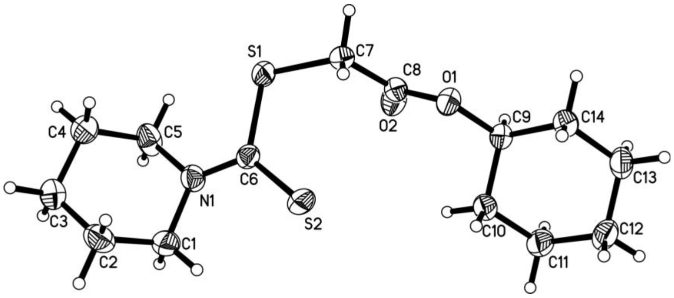


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Crystal data

$C_{14}H_{23}NO_2S_2$
$M_r = 301.47$
Triclinic, $P\overline{1}$
$a = 6.3643$ (1) Å
$b = 9.4441$ (2) Å
$c = 14.0709$ (5) Å
$\alpha = 102.332$ (2)°
$\beta = 96.380$ (2)°
$\gamma = 107.483$ (2)°
$V = 773.98$ (4) Å^3
$Z = 2$
$D_x = 1.294$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.34$ mm^{-1}
$T = 273$ (2) K
Block, colourless
0.47 × 0.36 × 0.26 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
5581 measured reflections
3039 independent reflections
2399 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\rm max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.096$
$S = 1.05$
3039 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.1538P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.25$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.25$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···S2$^{\rm i}$	0.97	2.94	3.7371 (18)	141

Symmetry code: (i) $x - 1, y, z$.

H atoms were placed in calculated positions with C—H = 0.97 or 0.98 Å and refined in riding mode, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Acta Cryst. (2007). E**63**, o200–o201 Cao *et al.* • $C_{14}H_{23}NO_2S_2$ **o201**