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N-Cyclohexylpyrrolidine-1-carbothioamide

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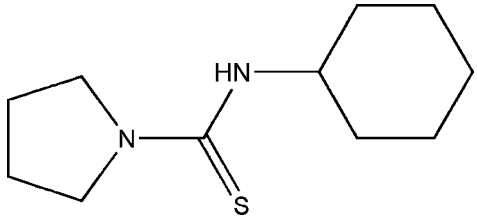
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.190; data-to-parameter ratio = 21.8.

In the title molecule, $C_{11}H_{20}N_2S$, the five-membered ring has an envelope conformation and the cyclohexane ring is in a chair conformation. The N—H group is not involved in any intra- or intermolecular interactions.

Related literature

For the medicinal properties of pyrrolidine compounds, see: Yang *et al.* (1997). For related structures, see: Köhn *et al.* (2004); Li (2011).



Experimental

Crystal data

$C_{11}H_{20}N_2S$
M_r = 212.35
Orthorhombic, *Pbca*
a = 9.3808 (19) Å
b = 10.925 (2) Å
c = 23.540 (5) Å
V = 2412.6 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 293 K
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
22078 measured reflections
2766 independent reflections
1700 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.190
S = 1.18
2766 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5439).

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supporting information

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N-Cyclohexylpyrrolidine-1-carbothioamide

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S1. Comment

Pyrrolidine compounds have been shown to have medicinal properties (Yang *et al.*, 1997). The molecular structure of the title compound is shown in Fig. 1. The five-membered ring has an envelope conformation with atom C2 forming the flap. The structures related compounds have been determined (Köhn *et al.*, 2004; Li, 2011).

S2. Experimental

A mixture of pyrrolidine (0.6 mol), and *N*-cyclohexylmethanethioamide (0.6 mol) was stirred in refluxing ethanol (14 ml) for 4 h to afford the title compound (0.51 mol, yield 85%). Colourless blocks of the title compound were obtained by recrystallization of a solution of the title compound ethanol at room temperature.

S3. Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93–0.97 Å; N—H = 0.86 Å and with U_{iso}(H) = 1.2U_{eq}(C,*N*).

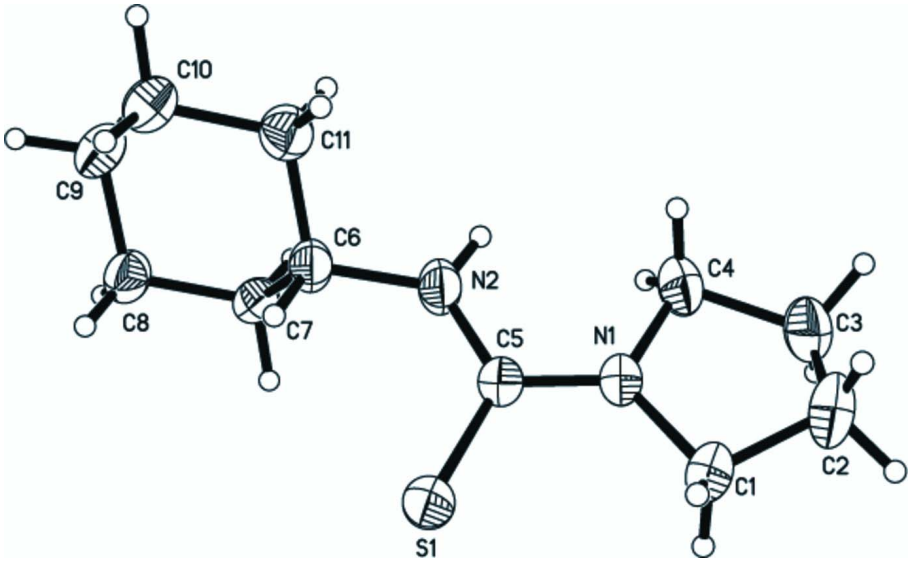

Figure 1

The molecular structure of the title compound showing 30% probability displacement ellipsoids.

N-Cyclohexylpyrrolidine-1-carbothioamide

Crystal data

$C_{11}H_{20}N_2S$
$M_r = 212.35$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 9.3808$ (19) Å
$b = 10.925$ (2) Å
$c = 23.540$ (5) Å
$V = 2412.6$ (8) Å^3
$Z = 8$
$F(000) = 928$
$D_x = 1.169$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1700 reflections
$\theta = 3.4$–$27.5°$
$\mu = 0.24$ mm^{-1}
$T = 293$ K
Block, colorless
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
22078 measured reflections
2766 independent reflections
1700 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 14$
$l = -30 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.190$
$S = 1.18$
2766 reflections
127 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1021P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.07717 (8)	0.34275 (5)	0.16033 (2)	0.0727 (3)
N2	0.1756 (2)	0.57053 (15)	0.14966 (7)	0.0649 (5)
H2A	0.2105	0.6354	0.1650	0.078*
N1	0.1569 (2)	0.49963 (16)	0.24023 (7)	0.0625 (5)
C5	0.1402 (2)	0.47798 (18)	0.18465 (8)	0.0533 (5)
C6	0.1600 (2)	0.57042 (18)	0.08782 (8)	0.0565 (6)

H6A	0.0941	0.5046	0.0773	0.068*
C7	0.3007 (3)	0.54772 (19)	0.05863 (8)	0.0604 (6)
H7A	0.3378	0.4686	0.0701	0.072*
H7B	0.3687	0.6098	0.0702	0.072*
C9	0.2197 (3)	0.6700 (2)	−0.02522 (9)	0.0637 (6)
H9A	0.2865	0.7359	−0.0179	0.076*
H9B	0.2032	0.6664	−0.0659	0.076*
C10	0.0817 (2)	0.6969 (2)	0.00449 (10)	0.0647 (6)
H10A	0.0103	0.6382	−0.0076	0.078*
H10B	0.0490	0.7778	−0.0064	0.078*
C11	0.0964 (2)	0.6912 (2)	0.06890 (10)	0.0657 (6)
H11A	0.1569	0.7578	0.0817	0.079*
H11B	0.0034	0.7015	0.0862	0.079*
C8	0.2838 (3)	0.5505 (2)	−0.00562 (8)	0.0655 (6)
H8A	0.3763	0.5396	−0.0233	0.079*
H8B	0.2230	0.4834	−0.0175	0.079*
C4	0.2130 (3)	0.6141 (2)	0.26409 (9)	0.0751 (7)
H4A	0.1503	0.6824	0.2557	0.090*
H4B	0.3073	0.6319	0.2493	0.090*
C3	0.2184 (4)	0.5887 (3)	0.32761 (10)	0.0947 (10)
H3A	0.3120	0.5596	0.3388	0.114*
H3B	0.1960	0.6619	0.3492	0.114*
C2	0.1095 (5)	0.4934 (3)	0.33665 (10)	0.1053 (11)
H2B	0.0163	0.5302	0.3418	0.126*
H2C	0.1320	0.4451	0.3700	0.126*
C1	0.1110 (4)	0.4151 (3)	0.28475 (9)	0.0917 (9)
H1A	0.1776	0.3477	0.2888	0.110*
H1B	0.0169	0.3826	0.2768	0.110*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.1120 (6)	0.0526 (4)	0.0536 (4)	−0.0127 (3)	−0.0018 (3)	−0.0005 (2)
N2	0.0950 (14)	0.0592 (11)	0.0406 (9)	−0.0187 (10)	0.0007 (8)	−0.0041 (7)
N1	0.0922 (14)	0.0560 (10)	0.0393 (9)	0.0013 (9)	0.0052 (9)	−0.0024 (7)
C5	0.0651 (13)	0.0519 (11)	0.0429 (10)	0.0033 (9)	0.0023 (9)	−0.0004 (8)
C6	0.0732 (14)	0.0557 (12)	0.0408 (10)	−0.0137 (10)	−0.0010 (9)	−0.0014 (8)
C7	0.0765 (14)	0.0565 (12)	0.0482 (11)	0.0150 (10)	−0.0002 (10)	0.0070 (9)
C9	0.0625 (14)	0.0741 (14)	0.0545 (12)	−0.0005 (10)	−0.0019 (10)	0.0182 (10)
C10	0.0600 (14)	0.0720 (14)	0.0620 (13)	0.0034 (11)	−0.0089 (10)	0.0097 (11)
C11	0.0650 (14)	0.0706 (14)	0.0617 (13)	0.0093 (11)	0.0000 (10)	−0.0031 (11)
C8	0.0774 (15)	0.0722 (14)	0.0468 (11)	0.0104 (12)	0.0073 (10)	0.0057 (10)
C4	0.1016 (19)	0.0753 (14)	0.0484 (12)	−0.0030 (14)	−0.0013 (12)	−0.0143 (11)
C3	0.139 (3)	0.096 (2)	0.0492 (13)	0.0122 (19)	−0.0130 (15)	−0.0142 (12)
C2	0.155 (3)	0.119 (3)	0.0421 (14)	0.003 (2)	0.0090 (15)	0.0021 (14)
C1	0.156 (3)	0.0742 (17)	0.0452 (13)	−0.0016 (16)	0.0119 (14)	0.0066 (11)

Geometric parameters (Å, º)

S1—C5	1.691 (2)	C10—H10A	0.9700
N2—C5	1.346 (3)	C10—H10B	0.9700
N2—C6	1.463 (2)	C11—H11A	0.9700
N2—H2A	0.8600	C11—H11B	0.9700
N1—C5	1.339 (3)	C8—H8A	0.9700
N1—C1	1.462 (3)	C8—H8B	0.9700
N1—C4	1.469 (3)	C4—C3	1.522 (3)
C6—C7	1.509 (3)	C4—H4A	0.9700
C6—C11	1.515 (3)	C4—H4B	0.9700
C6—H6A	0.9800	C3—C2	1.475 (4)
C7—C8	1.521 (3)	C3—H3A	0.9700
C7—H7A	0.9700	C3—H3B	0.9700
C7—H7B	0.9700	C2—C1	1.491 (4)
C9—C10	1.500 (3)	C2—H2B	0.9700
C9—C8	1.510 (3)	C2—H2C	0.9700
C9—H9A	0.9700	C1—H1A	0.9700
C9—H9B	0.9700	C1—H1B	0.9700
C10—C11	1.524 (3)		
C5—N2—C6	125.71 (17)	C10—C11—H11A	109.4
C5—N2—H2A	117.1	C6—C11—H11B	109.4
C6—N2—H2A	117.1	C10—C11—H11B	109.4
C5—N1—C1	123.67 (19)	H11A—C11—H11B	108.0
C5—N1—C4	124.49 (18)	C9—C8—C7	111.29 (18)
C1—N1—C4	111.69 (18)	C9—C8—H8A	109.4
N1—C5—N2	115.87 (18)	C7—C8—H8A	109.4
N1—C5—S1	121.75 (16)	C9—C8—H8B	109.4
N2—C5—S1	122.37 (15)	C7—C8—H8B	109.4
N2—C6—C7	111.45 (17)	H8A—C8—H8B	108.0
N2—C6—C11	109.34 (16)	N1—C4—C3	103.42 (19)
C7—C6—C11	110.72 (16)	N1—C4—H4A	111.1
N2—C6—H6A	108.4	C3—C4—H4A	111.1
C7—C6—H6A	108.4	N1—C4—H4B	111.1
C11—C6—H6A	108.4	C3—C4—H4B	111.1
C6—C7—C8	110.99 (18)	H4A—C4—H4B	109.0
C6—C7—H7A	109.4	C2—C3—C4	104.3 (2)
C8—C7—H7A	109.4	C2—C3—H3A	110.9
C6—C7—H7B	109.4	C4—C3—H3A	110.9
C8—C7—H7B	109.4	C2—C3—H3B	110.9
H7A—C7—H7B	108.0	C4—C3—H3B	110.9
C10—C9—C8	111.75 (18)	H3A—C3—H3B	108.9
C10—C9—H9A	109.3	C3—C2—C1	106.3 (2)
C8—C9—H9A	109.3	C3—C2—H2B	110.5
C10—C9—H9B	109.3	C1—C2—H2B	110.5
C8—C9—H9B	109.3	C3—C2—H2C	110.5
H9A—C9—H9B	107.9	C1—C2—H2C	110.5

C9—C10—C11	112.17 (18)	H2B—C2—H2C	108.7
C9—C10—H10A	109.2	N1—C1—C2	103.2 (2)
C11—C10—H10A	109.2	N1—C1—H1A	111.1
C9—C10—H10B	109.2	C2—C1—H1A	111.1
C11—C10—H10B	109.2	N1—C1—H1B	111.1
H10A—C10—H10B	107.9	C2—C1—H1B	111.1
C6—C11—C10	111.34 (18)	H1A—C1—H1B	109.1
C6—C11—H11A	109.4		