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N-Cyclopentyl-N-(3-oxo-2,3-dihydro-1H-inden-1-yl)acetamide

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N-Cyclopentyl-N-(3-oxo-2,3-dihydro-1H-inden-1-yl)acetamide

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The title molecule, C16H19NO2, consists of an indane moiety, which is connected through an N atom to an acetamide group and a cyclopentane ring. The N atom adopts planar triangular geometry. Intermolecular interactions, such as π–π stacking or hydrogen bonding, were not observed.

Related literature

For background information on the indane pharmacophore, see: Vaccva et al. (1994); Buckle et al. (1973); Heinzelmann et al. (1940). For details of the pharmacological activity of the title compound, see: Sheridan et al. (1990, 1999a,b, 2008); Frankish et al. (2004). For ionization characteristics, see: Simplicio et al. (2004).

Experimental

Crystal data

C16H19NO2
M_r = 257.32
Triclinic, P T

α = 87.97 (3)°
β = 81.29 (3)°
γ = 63.15 (3)°
V = 651.8 (2) Å³
Z = 2

α = 87.97 (3)°
β = 81.29 (3)°
γ = 63.15 (3)°
V = 651.8 (2) Å³
Z = 2

Mo Kα radiation
µ = 0.09 mm⁻¹
T = 150 K
0.60 × 0.50 × 0.30 mm

Data collection

Rigaku Saturn 724 diffractometer
Absorption correction: multi-scan
(CrystalClear; Rigaku, 2006)

T_mín = 0.726, T_máx = 1.000
μ = 0.100; data-to-parameter ratio = 12.6.

174 parameters
H-atom parameters constrained

Determination of the structure was carried out using CrystalClear (Rigaku, 2006); cell refinement: CrystalClear; data reduction: CrystalClear; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 1998); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5169).

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Comment

The indane pharmacophore occurs in many different bioactive molecules. Indinavir, a HIV-1 inhibitor is a protease inhibitor in clinical use that contains an indane fragment (Vacca et al., 1994). Nivemedone, a nitro-indanone has anti-allergenic activity (Buckle et al., 1973) while many simple indanols demonstrate bronchodilatory activity (Heinzelmann et al., 1940). We have demonstrated that indanone derivatives possess smooth muscle relaxant activity and inhibit mediator release (Sheridan et al., 1990, 1999a, 1999b; Frankish et al., 2004). In a recent study on bioactivity we evaluated the smooth muscle relaxant activity and mediator release inhibition activities demonstrated by a series of aminoindanones (Simplicio et al., 2004; Sheridan et al., 2008).

The asymmetric unit of the compound presented in this paper contains a single molecule of N-cyclopentyl-N-(3-oxo-2,3-dihydro-1H-inden-1-yl)acetamide. The geometry around the nitrogen atom can be best described as trigonal planar. As there are no flexible hydrogen atoms attached to the nitrogen atom N1 or the oxygen atoms (O1 and O2) hydrogen bonding do not prevail in the title compound. The shortest distance between the aromatic rings is 4.150 (9) Å and cannot be considered as the π-π stacking interaction.

The packing diagram of the structure, presented in Fig. 2, shows that the molecules are separated and when viewed along the crystallographic a-axis seem to form a sheet-like structure in the ab-plane. These sheets pack in the direction of the crystallographic c-axis. The shortest separation distance between them is 4.243 (75) Å and a weak Van der Vaals force or an electrostatic interaction may be responsible for holding the sheets together.

Experimental

The title compound was synthesized as reported (Sheridan et al., 2008). N-Bromosuccinimide (672 mg, 3.78 mmol) and a catalytic amount of dibenzoylperoxide were added to a solution of indan-1-one (500 mg, 3.78 mmol) in CCl₄ (15 ml) and the reaction was refluxed for 45 min. After cooling, the reaction was washed with water, dried over Na₂SO₄, filtered and evaporated in vacuo. The resultant was purified by column chromatography over silica gel (eluant, pet. ether:EtOAc, 4:1) to yield 3-bromoindan-1-one as an oil. To this 3-bromoindan-1-one solution (200 mg, 0.95 mmol) in dry DCM was added cyclopentanamine (80 mg, 0.94 mmol) and triethylamine (200 mg, 1.98 mmol). The reaction was stirred at 0°C for 3 h. The solvent was removed in vacuo and the residue was purified directly by flash column chromatography on silica gel (eluant, pet. ether:EtOAc, 4:1). After evaporation of the eluent the secondary amine was isolated as an oil (175 mg, 86%).

To this secondary amine solution (700 mg, 3.25 mmol) in DCM (5 ml) was added triethylamine (657 mg, 0.90 ml, 6.51 mmol), acetic anhydride (664 mg, 0.61 ml, 6.51 mmol) and DMAP (476 mg, 3.90 mmol). The reaction was stirred at room temperature for 2 h. The reaction mixture was then washed with water, dried over Na₂SO₄, filtered and evaporated in vacuo. The residue was purified by column chromatography over silica gel (pet. ether:EtOAc, 4:1) to yield the title compound as a white solid (450 mg, 54%). Crystals suitable for X-ray diffraction were obtained after 5 days of slow evaporation of an ethanol solution.
Refinement
All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å for aromatic H atoms, 0.96 Å for CH₃ type H atoms, 0.97 Å for CH₂ type H atoms and 0.98 Å for CH type H atoms, respectively. $U_{iso}(H)$ values were set at 1.5$U_{eq}(C)$ for methyl H atoms, and 1.2$U_{eq}(C)$ for the rest of the H atoms.

Computing details
Data collection: CrystalClear (Rigaku, 2006); cell refinement: CrystalClear (Rigaku, 2006); data reduction: CrystalClear (Rigaku, 2006); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 1998); software used to prepare material for publication: SHELXL97 (Sheldrick, 2008).

Figure 1
The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.
Figure 2
Packing diagram of the title compound viewed along the crystallographic a-axis.

N-Cyclopentyl-N-(3-oxo-2,3-dihydro-1H-inden-1-yl)acetamide

Crystal data
C₁₆H₁₉NO₂  
Mr = 257.32  
Triclinic, P1  
Hall symbol: -P 1  
a = 8.1539 (16) Å  
b = 8.9944 (18) Å  
c = 10.084 (2) Å  
α = 87.97 (3)°  
β = 81.29 (3)°  
γ = 63.15 (3)°  
V = 651.8 (2) Å³  
Z = 2  
F(000) = 276  
Dₐ = 1.311 Mg m⁻³  
Mo Kα radiation, λ = 0.71073 Å  
θ = 2.0–31.2°  
µ = 0.09 mm⁻¹  
T = 150 K  
Prism, colourless  
0.60 × 0.50 × 0.30 mm

Data collection
Rigaku Saturn 724 diffractometer  
Absorption correction: multi-scan  
(CrystalClear; Rigaku, 2006)  
Radiation source: fine-focus sealed tube  
Tₘᵢₘ = 0.726, Tₘₐₓ = 1.000  
Graphite monochromator  
7260 measured reflections  
Detector resolution: 28.5714 pixels mm⁻¹  
2191 independent reflections  
ω and phi scans  
2157 reflections with I > 2σ(I)  
Rₑₘ = 0.026
\[ \theta_{\text{max}} = 25.0^\circ, \theta_{\text{min}} = 2.8^\circ \]
\[ k = -10 \rightarrow 8 \]
\[ l = -11 \rightarrow 11 \]

**Refinement**

Refinement on \( F^2 \)

Least-squares matrix: full

\[ R(F^2 > 2\sigma(F^2)) = 0.042 \]
\[ wR(F^2) = 0.100 \]
\[ S = 1.13 \]

2191 reflections

174 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

\[ w = 1/\left[ \sigma^2(F_o^2) + (0.0406P)^2 + 0.3106P \right] \]

\[ (\Delta\sigma)_{\text{max}} < 0.001 \]

\[ \Delta \rho_{\text{max}} = 0.21 \text{ e\ Å}^{-3} \]
\[ \Delta \rho_{\text{min}} = -0.23 \text{ e\ Å}^{-3} \]

**Special details**

**Experimental.** The su's on the Cell Angles were measured.

**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 considering all data 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       | \( U_{\text{iso}}^* \)/\( U_{\text{eq}} \) |
|---------|---------|---------|-----------------------------------|
| O2      | 0.13603 (15) | 0.52993 (14) | 0.35282 (11) | 0.0247 (3) |
| N1      | 0.26193 (16) | 0.31399 (15) | 0.30730 (12) | 0.0180 (3) |
| C12     | 0.3026 (2)   | 0.13741 (18) | 0.31299 (14) | 0.0178 (3) |
| H12     | 0.4075      | 0.0812     | 0.3627     | 0.021* |
| C5      | 0.15437 (19) | 0.51234 (18) | 0.12014 (14) | 0.0178 (3) |
| C9      | 0.10493 (19) | 0.42530 (18) | 0.24012 (14) | 0.0182 (3) |
| H9      | 0.0535      | 0.3566     | 0.2071     | 0.022* |
| C6      | 0.0277 (2)   | 0.67950 (19) | 0.12237 (14) | 0.0188 (3) |
| C10     | 0.3582 (2)   | 0.38022 (19) | 0.36131 (14) | 0.0191 (3) |
| C4      | 0.2976 (2)   | 0.4435 (2)  | 0.01256 (15) | 0.0221 (3) |
| H4      | 0.3821      | 0.3311     | 0.0095     | 0.027* |
| C7      | -0.1091 (2)  | 0.72363 (19) | 0.24640 (15) | 0.0199 (3) |
| C11     | 0.5168 (2)   | 0.2668 (2)  | 0.43334 (16) | 0.0245 (4) |
| H11A    | 0.5711      | 0.3301     | 0.4669     | 0.037* |
| H11B    | 0.6092      | 0.1799     | 0.3720     | 0.037* |
| H11C    | 0.4709      | 0.2182     | 0.5069     | 0.037* |
| C1      | 0.0406 (2)   | 0.7826 (2)  | 0.01944 (15) | 0.0226 (3) |
| H1      | -0.0454     | 0.8945     | 0.0219     | 0.027* |
| C16     | 0.1404 (2)   | 0.10622 (19) | 0.38594 (15) | 0.0222 (3) |
| H16A    | 0.1517      | 0.0863     | 0.4801     | 0.027* |
| H16B    | 0.0218      | 0.2016     | 0.3793     | 0.027* |
| C13     | 0.3576 (2)   | 0.04558 (19) | 0.17613 (14) | 0.0205 (3) |
| H13A    | 0.2763      | 0.1118     | 0.1132     | 0.025* |
supplementary materials

| Atom  | x    | y    | z    | U11  | U22  | U33  | U12  | U13  | U23  |
|-------|------|------|------|------|------|------|------|------|------|
| H13B  | 0.4852 | 0.0175 | 0.1386 | 0.025* |
| C3    | 0.3120 (2) | 0.5459 (2) | -0.09033 (15) | 0.0245 (4) |
| H3    | 0.4079 | 0.5014 | -0.1624 | 0.029* |
| C14   | 0.3337 (2) | -0.11046 (19) | 0.21048 (15) | 0.0227 (3) |
| H14A  | 0.4397 | -0.1927 | 0.2482 | 0.027* |
| H14B  | 0.3200 | -0.1595 | 0.1313 | 0.027* |
| C2    | 0.1849 (2) | 0.7143 (2) | -0.08713 (15) | 0.0251 (4) |
| H2    | 0.1969 | 0.7811 | -0.1566 | 0.030* |
| C8    | -0.0572 (2) | 0.56929 (19) | 0.32894 (15) | 0.0223 (3) |
| H8A   | -0.1624 | 0.5451 | 0.3517 | 0.027* |
| H8B   | -0.0181 | 0.5849 | 0.4113 | 0.027* |
| C15   | 0.1556 (2) | -0.04907 (19) | 0.31440 (16) | 0.0242 (4) |
| H15A  | 0.1640 | -0.1346 | 0.3782 | 0.029* |
| H15B  | 0.0478 | -0.0206 | 0.2704 | 0.029* |
| O1    | -0.24001 (15) | 0.85977 (14) | 0.27869 (11) | 0.0280 (3) |

Atomic displacement parameters (Å²)

|       | U11  | U22  | U33  | U12  | U13  | U23  |
|-------|------|------|------|------|------|------|
| O2    | 0.0310 (6) | 0.0181 (7) | 0.0266 (6) | -0.0122 (5) | -0.0055 (5) | 0.0010 (4) |
| N1    | 0.0186 (6) | 0.0145 (7) | 0.0187 (6) | -0.0058 (5) | -0.0023 (5) | 0.0003 (5) |
| C12   | 0.0196 (7) | 0.0130 (8) | 0.0187 (7) | -0.0058 (6) | -0.0016 (6) | 0.0001 (6) |
| C5    | 0.0174 (7) | 0.0187 (8) | 0.0181 (7) | -0.0083 (6) | -0.0052 (5) | 0.0009 (6) |
| C9    | 0.0168 (7) | 0.0159 (8) | 0.0192 (7) | -0.0055 (6) | -0.0011 (5) | -0.0003 (6) |
| C6    | 0.0187 (7) | 0.0180 (8) | 0.0213 (7) | -0.0083 (6) | -0.0072 (6) | 0.0007 (6) |
| C10   | 0.0206 (7) | 0.0199 (9) | 0.0154 (7) | -0.0089 (6) | 0.0008 (5) | -0.0016 (6) |
| C4    | 0.0209 (7) | 0.0201 (9) | 0.0225 (8) | -0.0071 (6) | -0.0021 (6) | -0.0006 (6) |
| C7    | 0.0164 (7) | 0.0190 (9) | 0.0235 (8) | -0.0063 (6) | -0.0054 (6) | -0.0029 (6) |
| C11   | 0.0248 (8) | 0.0229 (9) | 0.0271 (8) | -0.0108 (7) | -0.0072 (6) | -0.0002 (6) |
| C1    | 0.0235 (8) | 0.0192 (8) | 0.0266 (8) | -0.0096 (6) | -0.0092 (6) | 0.0030 (6) |
| C16   | 0.0236 (8) | 0.0196 (9) | 0.0212 (7) | -0.0092 (7) | 0.0017 (6) | -0.0008 (6) |
| C13   | 0.0188 (7) | 0.0199 (9) | 0.0192 (7) | -0.0061 (6) | -0.0007 (6) | -0.0021 (6) |
| C3    | 0.0239 (8) | 0.0313 (10) | 0.0192 (8) | -0.0136 (7) | -0.0019 (6) | 0.0000 (6) |
| C14   | 0.0220 (8) | 0.0186 (9) | 0.0255 (8) | -0.0071 (7) | -0.0032 (6) | -0.0044 (6) |
| C2    | 0.0306 (8) | 0.0299 (10) | 0.0211 (8) | -0.0181 (8) | -0.0091 (6) | 0.0079 (6) |
| C8    | 0.0189 (7) | 0.0206 (9) | 0.0218 (8) | -0.0051 (6) | 0.0008 (6) | -0.0015 (6) |
| C15   | 0.0235 (8) | 0.0183 (9) | 0.0304 (8) | -0.0098 (7) | -0.0010 (6) | -0.0012 (6) |
| O1    | 0.0219 (6) | 0.0211 (7) | 0.0327 (6) | -0.0026 (5) | -0.0025 (5) | -0.0031 (5) |

Geometric parameters (Å, °)

|       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|
| O2—C10 | 1.2334 (19) | C11—H11B | 0.9600 |
| N1—C10 | 1.3571 (19) | C11—H11C | 0.9600 |
| N1—C9  | 1.4687 (19) | C1—C2  | 1.389 (2) |
| N1—C12 | 1.470 (2)   | C1—H1  | 0.9300 |
| C12—C13 | 1.532 (2) | C16—C15 | 1.541 (2) |
| C12—C16 | 1.548 (2) | C16—H16A | 0.9700 |
| C12—H12 | 0.9800 | C16—H16B | 0.9700 |
| C5—C6  | 1.386 (2)   | C13—C14 | 1.523 (2) |
| C5—C4  | 1.391 (2)   | C13—H13A | 0.9700 |
C5—C9 & 1.520 (2) & C13—H13B & 0.9700  
C9—C8 & 1.551 (2) & C3—C2 & 1.394 (2)  
C9—H9 & 0.9800 & C3—H3 & 0.9300  
C6—C1 & 1.391 (2) & C14—C15 & 1.539 (2)  
C6—C7 & 1.476 (2) & C14—H14A & 0.9700  
C10—C11 & 1.511 (2) & C14—H14B & 0.9700  
C4—C3 & 1.390 (2) & C2—H2 & 0.9300  
C4—H4 & 0.9300 & C8—H8A & 0.9700  
C7—O1 & 1.2196 (19) & C8—H8B & 0.9700  
C7—C8 & 1.514 (2) & C14—C13—C12 & 112.50 (12)  
C11—H11A & 0.9600 & C14—C13—H13A & 111.3  
C11—H11B & 109.5 & C14—C13—H13B & 111.3  
C10—N1—C9 & 118.39 (12) & C12—C13—H13A & 111.3  
C10—N1—C12 & 124.30 (12) & C12—C13—H13B & 111.3  
C9—N1—C12 & 117.30 (12) & C16—C15—C16 & 104.59 (12)  
N1—C12—C13 & 105.21 (12) & C16—C15—H15A & 110.6  
N1—C12—C16 & 107.3 & C16—C15—H15B & 110.6  
N1—C12—H12 & 107.3 & C14—C13—C12 & 104.59 (12)  
C13—C12—C16 & 107.3 & C14—C13—H13A & 111.3  
C16—C12—C13 & 107.3 & C14—C13—H13B & 111.3  
C6—C5—C4 & 120.02 (14) & C16—C15—H15B & 110.6  
C6—C5—C9 & 111.41 (13) & C14—C13—H13B & 111.3  
C4—C5—C9 & 128.47 (14) & C14—C13—H13B & 111.3  
N1—C9—C5 & 115.14 (12) & C14—C13—H13B & 111.3  
N1—C9—C8 & 115.99 (12) & C14—C13—H13B & 111.3  
C5—C9—C8 & 103.95 (12) & C14—C13—H13B & 111.3  
N1—C9—H9 & 107.1 & C14—C13—H13B & 111.3  
C5—C9—H9 & 107.1 & C14—C13—H13B & 111.3  
C8—C9—H9 & 107.1 & C14—C13—H13B & 111.3  
C5—C6—C1 & 121.56 (14) & C14—C13—H13B & 111.3  
C5—C6—C7 & 110.07 (13) & C14—C13—H13B & 111.3  
C1—C6—C7 & 128.36 (14) & C14—C13—H13B & 111.3  
O2—C10—N1 & 120.77 (14) & C14—C13—H13B & 111.3  
O2—C10—C11 & 120.75 (13) & C14—C13—H13B & 111.3  
N1—C10—C11 & 118.48 (13) & C14—C13—H13B & 111.3  
C3—C4—C5 & 118.77 (15) & C14—C13—H13B & 111.3  
C3—C4—H4 & 120.6 & C14—C13—H13B & 111.3  
C5—C4—H4 & 120.6 & C14—C13—H13B & 111.3  
O1—C7—C6 & 126.77 (15) & C14—C13—H13B & 111.3  
O1—C7—C8 & 125.44 (14) & C14—C13—H13B & 111.3  
C6—C7—C8 & 107.79 (13) & C14—C13—H13B & 111.3  
C10—C11—H11A & 109.5 & C14—C13—H13B & 111.3  
C10—C11—H11B & 109.5 & C14—C13—H13B & 111.3  
H11A—C11—H11B & 109.5 & C14—C13—H13B & 111.3  
C10—C11—H11C & 109.5 & C14—C13—H13B & 111.3  
H11A—C11—H11C & 109.5 & C14—C13—H13B & 111.3  
H11B—C11—H11C & 109.5 & C14—C13—H13B & 111.3  
C2—C1—C6 & 118.40 (15) & C14—C13—H13B & 111.3  

*Acta Cryst. (2012). E68, o958*
C2—C1—H1 120.8

| Bond/Rotation Angle | Value (°) |
|---------------------|-----------|
| C10—N1—C12—C13     | -118.48 (15) |
| C9—N1—C12—C13      | 62.40 (16)   |
| C10—N1—C12—C16     | 119.67 (15)  |
| C9—N1—C12—C16      | -59.45 (16)  |
| C10—N1—C9—C5       | 60.63 (17)   |
| C12—N1—C9—C5       | -120.20 (14) |
| C10—N1—C9—C8       | -61.05 (17)  |
| C12—N1—C9—C8       | 118.12 (14)  |
| C6—C5—C9—N1        | -135.65 (13) |
| C4—C5—C9—N1        | 48.1 (2)     |
| C6—C5—C9—C8        | -7.66 (16)   |
| C4—C5—C9—C8        | 176.08 (14)  |
| C4—C6—C1            | -0.7 (2)     |
| C4—C6—C7            | -179.41 (12) |
| C9—C5—C6—C7        | 3.98 (16)    |
| C9—N1—C10—O2       | -0.8 (2)     |
| C12—N1—C10—O2      | -179.91 (12) |
| C9—N1—C10—C11      | 178.57 (12)  |
| C12—N1—C10—C11     | -0.5 (2)     |
| C6—C5—C4—C3        | 1.0 (2)      |