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# 1-Tetradecylindoline-2,3-dione

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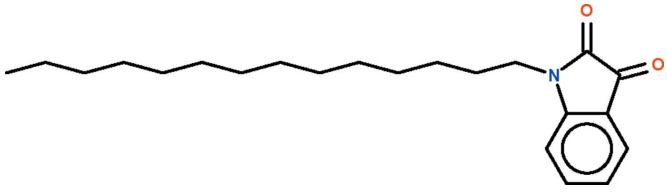
Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.065; $wR$ factor = 0.222; data-to-parameter ratio = 22.9.

In the title $N$-alkyl isatin, $C_{22}H_{33}NO_2$, the isatin moiety is planar (r.m.s. deviation = 0.03 Å). The tetradecyl substituent has all torsion angles in an antiperiplanar conformation.

## Related literature

For background to $N$-substituted isatins and their derivatives, see: Bouhfid *et al.* (2008). For the crystal structures of two $N$-alkyl isatins, see: Miehe *et al.* (2003); Naumov *et al.* (2002).




## Experimental

### *Crystal data*

$C_{22}H_{33}NO_2$ $M_r$ = 343.49
Monoclinic, $P2_1/c$
$a$ = 27.6647 (8) Å
$b$ = 4.7055 (1) Å
$c$ = 15.7583 (5) Å
$\beta$ = 103.635 (1)°
$V$ = 1993.54 (10) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 200 K
0.18 × 0.16 × 0.11 mm

### *Data collection*

Bruker X8 APEXII diffractometer
23477 measured reflections
5172 independent reflections
3532 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.222
$S$ = 1.11
5172 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5273).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o1410 [ **doi:10.1107/S1600536810018258** ]

# 1-Tetradecylindoline-2,3-dione

**K. Mamari, H. Zouihri, E. M. Essassi and S. W. Ng**

## Comment

*N*-Substituted isatins (Bouhfid *et al.*, 2008) represent a large family of heterocyclic compounds reported to show a wide range of useful medicinal activities. These are readily synthesized by the reaction of isatin and an alkyl halide in the presence of a catalyst. The title tetradecyl derivative (Scheme I, Fig. 1) has a particarly long hydrocarbon chain; the chain adopts a extended zigzag conformation.

The crystal structures of only few *N*-substituted isatins have been reported; these have only short hydrocarbon chains, e.g., methyl isatin (Miehe *et al.*, 2003) and ethyl isatin (Naumov *et al.*, 2002).

## Experimental

To a solution of isatin (1 g, 6.8 mmol) dissolved in DMF(50 ml) was added 1-bromotetradecane (1.87 g, 6.8 mmol), potassium carbonate (1 g, 7.4 mmol) and a catalytic quantity of tetra-*n*-butylammonium bromide.The mixture was stirred for 48 h; the reaction was monitored by thin layer chromatography. The mixture was filtered and the solvent removed under vacuum. The solid that was obtained was recrystallized from ethanol to afford the title compound as orange crystals in 80% yield.

## Refinement

H-atoms were placed in calculated positions (C–H 0.95–0.99 Å) and were included in the refinement in the riding model approximation, with $U$(H) set to 1.2–1.5$U_{eq}$(C).

## Figures

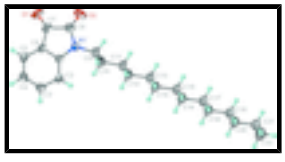


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of the title compound at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

## 1-Tetradecylindoline-2,3-dione

*Crystal data*

| | |
|---|---|
| $C_{22}H_{33}NO_2$ | $F$(000) = 752 |
| $M_r$ = 343.49 | $D_x$ = 1.144 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 4926 reflections |
| $a$ = 27.6647 (8) Å | θ = 2.6–28.7° |

| | |
|---|---|
| $b$ = 4.7055 (1) Å | μ = 0.07 mm$^{-1}$ |
| $c$ = 15.7583 (5) Å | $T$ = 200 K |
| β = 103.635 (1)° | Irregular block, orange |
| $V$ = 1993.54 (10) Å$^3$ | 0.18 × 0.16 × 0.11 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker X8 APEXII diffractometer | 3532 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.042 |
| graphite | $\theta_{max}$ = 28.8°, $\theta_{min}$ = 2.3° |
| φ and ω scans | $h$ = −37→37 |
| 23477 measured reflections | $k$ = −6→5 |
| 5172 independent reflections | $l$ = −21→21 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.065 | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2)$ = 0.222 | H-atom parameters constrained |
| $S$ = 1.11 | $w = 1/[\sigma^2(F_o^2) + (0.098P)^2 + 1.1616P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 5172 reflections | $(\Delta/\sigma)_{max}$ = 0.001 |
| 226 parameters | $\Delta\rho_{max}$ = 0.27 e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min}$ = −0.20 e Å$^{-3}$ |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.46046 (6) | 1.1884 (4) | 0.43051 (11) | 0.0487 (5) |
| O2 | 0.38053 (7) | 0.7712 (5) | 0.36601 (11) | 0.0524 (5) |
| N1 | 0.37452 (6) | 0.7894 (4) | 0.50944 (11) | 0.0309 (4) |
| C1 | 0.39707 (7) | 0.9506 (4) | 0.58407 (12) | 0.0263 (4) |
| C2 | 0.38674 (7) | 0.9454 (5) | 0.66525 (13) | 0.0312 (4) |
| H2 | 0.3623 | 0.8214 | 0.6780 | 0.037* |
| C3 | 0.41379 (8) | 1.1306 (5) | 0.72815 (14) | 0.0352 (5) |
| H3 | 0.4073 | 1.1327 | 0.7847 | 0.042* |
| C4 | 0.44969 (8) | 1.3112 (5) | 0.71059 (15) | 0.0376 (5) |
| H4 | 0.4672 | 1.4355 | 0.7548 | 0.045* |
| C5 | 0.46031 (7) | 1.3115 (5) | 0.62847 (14) | 0.0339 (5) |
| H5 | 0.4852 | 1.4326 | 0.6160 | 0.041* |
| C6 | 0.43356 (7) | 1.1305 (4) | 0.56570 (12) | 0.0282 (4) |
| C7 | 0.43501 (7) | 1.0834 (5) | 0.47474 (13) | 0.0339 (5) |
| C8 | 0.39388 (8) | 0.8608 (5) | 0.43985 (14) | 0.0352 (5) |

| | | | | |
|---|---|---|---|---|
| C9 | 0.33228 (7) | 0.5996 (5) | 0.50282 (16) | 0.0354 (5) |
| H9A | 0.3371 | 0.4853 | 0.5569 | 0.042* |
| H9B | 0.3306 | 0.4673 | 0.4534 | 0.042* |
| C10 | 0.28326 (7) | 0.7629 (5) | 0.48906 (15) | 0.0342 (5) |
| H10A | 0.2832 | 0.8755 | 0.5421 | 0.041* |
| H10B | 0.2808 | 0.8974 | 0.4399 | 0.041* |
| C11 | 0.23799 (7) | 0.5690 (5) | 0.46968 (15) | 0.0341 (5) |
| H11A | 0.2405 | 0.4329 | 0.5185 | 0.041* |
| H11B | 0.2377 | 0.4583 | 0.4161 | 0.041* |
| C12 | 0.18917 (7) | 0.7341 (5) | 0.45715 (15) | 0.0346 (5) |
| H12A | 0.1886 | 0.8336 | 0.5123 | 0.042* |
| H12B | 0.1880 | 0.8803 | 0.4115 | 0.042* |
| C13 | 0.14296 (7) | 0.5478 (5) | 0.43108 (15) | 0.0347 (5) |
| H13A | 0.1440 | 0.4011 | 0.4765 | 0.042* |
| H13B | 0.1433 | 0.4492 | 0.3757 | 0.042* |
| C14 | 0.09459 (7) | 0.7159 (5) | 0.41929 (15) | 0.0359 (5) |
| H14A | 0.0941 | 0.8117 | 0.4750 | 0.043* |
| H14B | 0.0939 | 0.8651 | 0.3748 | 0.043* |
| C15 | 0.04810 (7) | 0.5345 (5) | 0.39165 (15) | 0.0364 (5) |
| H15A | 0.0487 | 0.3850 | 0.4361 | 0.044* |
| H15B | 0.0485 | 0.4391 | 0.3358 | 0.044* |
| C16 | 0.00019 (7) | 0.7038 (5) | 0.38033 (15) | 0.0373 (5) |
| H16A | −0.0003 | 0.8538 | 0.3361 | 0.045* |
| H16B | −0.0001 | 0.7987 | 0.4363 | 0.045* |
| C17 | −0.04666 (7) | 0.5241 (5) | 0.35234 (15) | 0.0376 (5) |
| H17A | −0.0463 | 0.3745 | 0.3967 | 0.045* |
| H17B | −0.0463 | 0.4288 | 0.2965 | 0.045* |
| C18 | −0.09460 (7) | 0.6944 (5) | 0.34082 (16) | 0.0377 (5) |
| H18A | −0.0948 | 0.7913 | 0.3965 | 0.045* |
| H18B | −0.0951 | 0.8430 | 0.2961 | 0.045* |
| C19 | −0.14159 (7) | 0.5157 (6) | 0.31364 (16) | 0.0386 (5) |
| H19A | −0.1415 | 0.4188 | 0.2579 | 0.046* |
| H19B | −0.1411 | 0.3672 | 0.3583 | 0.046* |
| C20 | −0.18930 (8) | 0.6862 (6) | 0.30219 (16) | 0.0390 (5) |
| H20A | −0.1894 | 0.7831 | 0.3579 | 0.047* |
| H20B | −0.1897 | 0.8348 | 0.2575 | 0.047* |
| C21 | −0.23622 (8) | 0.5095 (6) | 0.27508 (17) | 0.0447 (6) |
| H21A | −0.2358 | 0.3606 | 0.3196 | 0.054* |
| H21B | −0.2363 | 0.4133 | 0.2192 | 0.054* |
| C22 | −0.28379 (8) | 0.6818 (7) | 0.2641 (2) | 0.0543 (7) |
| H22A | −0.3126 | 0.5554 | 0.2469 | 0.081* |
| H22B | −0.2850 | 0.8263 | 0.2188 | 0.081* |
| H22C | −0.2844 | 0.7747 | 0.3195 | 0.081* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0391 (9) | 0.0730 (13) | 0.0381 (9) | 0.0013 (9) | 0.0171 (7) | 0.0179 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O2 | 0.0500 (10) | 0.0715 (13) | 0.0335 (9) | 0.0075 (10) | 0.0056 (7) | −0.0139 (8) |
| N1 | 0.0226 (8) | 0.0361 (10) | 0.0329 (9) | −0.0005 (7) | 0.0045 (7) | −0.0041 (7) |
| C1 | 0.0209 (8) | 0.0309 (10) | 0.0261 (9) | 0.0024 (8) | 0.0035 (7) | 0.0019 (8) |
| C2 | 0.0268 (9) | 0.0377 (11) | 0.0301 (10) | −0.0018 (9) | 0.0087 (8) | 0.0045 (8) |
| C3 | 0.0351 (11) | 0.0438 (13) | 0.0269 (10) | 0.0039 (10) | 0.0078 (8) | 0.0003 (9) |
| C4 | 0.0347 (11) | 0.0366 (12) | 0.0382 (11) | −0.0014 (10) | 0.0023 (9) | −0.0041 (9) |
| C5 | 0.0246 (9) | 0.0355 (11) | 0.0398 (11) | −0.0036 (9) | 0.0041 (8) | 0.0047 (9) |
| C6 | 0.0222 (9) | 0.0337 (11) | 0.0287 (9) | 0.0030 (8) | 0.0060 (7) | 0.0067 (8) |
| C7 | 0.0256 (9) | 0.0451 (13) | 0.0314 (10) | 0.0094 (9) | 0.0073 (8) | 0.0121 (9) |
| C8 | 0.0297 (10) | 0.0450 (13) | 0.0301 (10) | 0.0104 (10) | 0.0055 (8) | −0.0007 (9) |
| C9 | 0.0223 (9) | 0.0332 (11) | 0.0478 (12) | −0.0004 (9) | 0.0026 (8) | −0.0053 (9) |
| C10 | 0.0227 (9) | 0.0297 (11) | 0.0475 (12) | −0.0006 (8) | 0.0030 (9) | −0.0047 (9) |
| C11 | 0.0208 (9) | 0.0342 (11) | 0.0450 (12) | 0.0001 (8) | 0.0032 (8) | −0.0041 (9) |
| C12 | 0.0217 (9) | 0.0344 (11) | 0.0457 (12) | 0.0001 (8) | 0.0036 (8) | −0.0026 (9) |
| C13 | 0.0208 (9) | 0.0390 (12) | 0.0423 (11) | −0.0007 (9) | 0.0035 (8) | −0.0028 (9) |
| C14 | 0.0218 (9) | 0.0404 (12) | 0.0443 (12) | 0.0005 (9) | 0.0056 (8) | −0.0012 (10) |
| C15 | 0.0220 (9) | 0.0432 (13) | 0.0425 (12) | −0.0004 (9) | 0.0044 (9) | −0.0026 (10) |
| C16 | 0.0225 (9) | 0.0424 (13) | 0.0456 (12) | 0.0003 (9) | 0.0055 (9) | −0.0017 (10) |
| C17 | 0.0225 (9) | 0.0447 (13) | 0.0439 (12) | −0.0001 (9) | 0.0042 (9) | −0.0038 (10) |
| C18 | 0.0211 (9) | 0.0437 (13) | 0.0460 (12) | 0.0001 (9) | 0.0032 (9) | −0.0012 (10) |
| C19 | 0.0228 (9) | 0.0474 (14) | 0.0442 (12) | 0.0003 (9) | 0.0050 (9) | −0.0048 (10) |
| C20 | 0.0237 (10) | 0.0454 (13) | 0.0458 (12) | 0.0004 (10) | 0.0042 (9) | −0.0012 (10) |
| C21 | 0.0277 (11) | 0.0535 (15) | 0.0508 (14) | −0.0028 (11) | 0.0052 (10) | −0.0085 (12) |
| C22 | 0.0246 (11) | 0.0702 (19) | 0.0649 (17) | −0.0010 (12) | 0.0045 (11) | −0.0017 (15) |

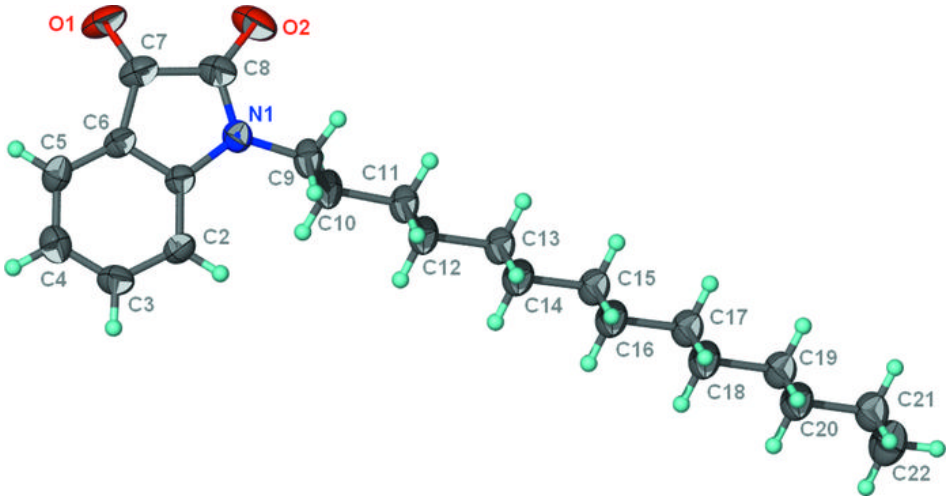
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.207 (2) | C13—H13A | 0.9900 |
| O2—C8 | 1.211 (3) | C13—H13B | 0.9900 |
| N1—C8 | 1.371 (3) | C14—C15 | 1.519 (3) |
| N1—C1 | 1.415 (3) | C14—H14A | 0.9900 |
| N1—C9 | 1.455 (3) | C14—H14B | 0.9900 |
| C1—C2 | 1.375 (3) | C15—C16 | 1.520 (3) |
| C1—C6 | 1.399 (3) | C15—H15A | 0.9900 |
| C2—C3 | 1.397 (3) | C15—H15B | 0.9900 |
| C2—H2 | 0.9500 | C16—C17 | 1.523 (3) |
| C3—C4 | 1.384 (3) | C16—H16A | 0.9900 |
| C3—H3 | 0.9500 | C16—H16B | 0.9900 |
| C4—C5 | 1.393 (3) | C17—C18 | 1.523 (3) |
| C4—H4 | 0.9500 | C17—H17A | 0.9900 |
| C5—C6 | 1.381 (3) | C17—H17B | 0.9900 |
| C5—H5 | 0.9500 | C18—C19 | 1.522 (3) |
| C6—C7 | 1.460 (3) | C18—H18A | 0.9900 |
| C7—C8 | 1.549 (3) | C18—H18B | 0.9900 |
| C9—C10 | 1.529 (3) | C19—C20 | 1.519 (3) |
| C9—H9A | 0.9900 | C19—H19A | 0.9900 |
| C9—H9B | 0.9900 | C19—H19B | 0.9900 |
| C10—C11 | 1.521 (3) | C20—C21 | 1.516 (3) |
| C10—H10A | 0.9900 | C20—H20A | 0.9900 |

| | | | |
|---|---|---|---|
| C10—H10B | 0.9900 | C20—H20B | 0.9900 |
| C11—C12 | 1.530 (3) | C21—C22 | 1.520 (3) |
| C11—H11A | 0.9900 | C21—H21A | 0.9900 |
| C11—H11B | 0.9900 | C21—H21B | 0.9900 |
| C12—C13 | 1.524 (3) | C22—H22A | 0.9800 |
| C12—H12A | 0.9900 | C22—H22B | 0.9800 |
| C12—H12B | 0.9900 | C22—H22C | 0.9800 |
| C13—C14 | 1.527 (3) | | |
| C8—N1—C1 | 110.78 (17) | H13A—C13—H13B | 107.8 |
| C8—N1—C9 | 123.48 (18) | C15—C14—C13 | 113.71 (19) |
| C1—N1—C9 | 125.31 (17) | C15—C14—H14A | 108.8 |
| C2—C1—C6 | 121.43 (19) | C13—C14—H14A | 108.8 |
| C2—C1—N1 | 128.04 (18) | C15—C14—H14B | 108.8 |
| C6—C1—N1 | 110.53 (16) | C13—C14—H14B | 108.8 |
| C1—C2—C3 | 117.06 (19) | H14A—C14—H14B | 107.7 |
| C1—C2—H2 | 121.5 | C14—C15—C16 | 113.3 (2) |
| C3—C2—H2 | 121.5 | C14—C15—H15A | 108.9 |
| C4—C3—C2 | 122.05 (19) | C16—C15—H15A | 108.9 |
| C4—C3—H3 | 119.0 | C14—C15—H15B | 108.9 |
| C2—C3—H3 | 119.0 | C16—C15—H15B | 108.9 |
| C3—C4—C5 | 120.3 (2) | H15A—C15—H15B | 107.7 |
| C3—C4—H4 | 119.8 | C15—C16—C17 | 113.7 (2) |
| C5—C4—H4 | 119.8 | C15—C16—H16A | 108.8 |
| C6—C5—C4 | 118.04 (19) | C17—C16—H16A | 108.8 |
| C6—C5—H5 | 121.0 | C15—C16—H16B | 108.8 |
| C4—C5—H5 | 121.0 | C17—C16—H16B | 108.8 |
| C5—C6—C1 | 121.07 (18) | H16A—C16—H16B | 107.7 |
| C5—C6—C7 | 131.52 (19) | C16—C17—C18 | 113.6 (2) |
| C1—C6—C7 | 107.41 (18) | C16—C17—H17A | 108.8 |
| O1—C7—C6 | 131.3 (2) | C18—C17—H17A | 108.8 |
| O1—C7—C8 | 123.5 (2) | C16—C17—H17B | 108.8 |
| C6—C7—C8 | 105.27 (16) | C18—C17—H17B | 108.8 |
| O2—C8—N1 | 126.5 (2) | H17A—C17—H17B | 107.7 |
| O2—C8—C7 | 127.5 (2) | C19—C18—C17 | 113.9 (2) |
| N1—C8—C7 | 105.93 (17) | C19—C18—H18A | 108.8 |
| N1—C9—C10 | 111.84 (18) | C17—C18—H18A | 108.8 |
| N1—C9—H9A | 109.2 | C19—C18—H18B | 108.8 |
| C10—C9—H9A | 109.2 | C17—C18—H18B | 108.8 |
| N1—C9—H9B | 109.2 | H18A—C18—H18B | 107.7 |
| C10—C9—H9B | 109.2 | C20—C19—C18 | 113.7 (2) |
| H9A—C9—H9B | 107.9 | C20—C19—H19A | 108.8 |
| C11—C10—C9 | 112.80 (18) | C18—C19—H19A | 108.8 |
| C11—C10—H10A | 109.0 | C20—C19—H19B | 108.8 |
| C9—C10—H10A | 109.0 | C18—C19—H19B | 108.8 |
| C11—C10—H10B | 109.0 | H19A—C19—H19B | 107.7 |
| C9—C10—H10B | 109.0 | C21—C20—C19 | 114.0 (2) |
| H10A—C10—H10B | 107.8 | C21—C20—H20A | 108.8 |
| C10—C11—C12 | 112.39 (18) | C19—C20—H20A | 108.8 |
| C10—C11—H11A | 109.1 | C21—C20—H20B | 108.8 |

| | | | |
|---|---|---|---|
| C12—C11—H11A | 109.1 | C19—C20—H20B | 108.8 |
| C10—C11—H11B | 109.1 | H20A—C20—H20B | 107.7 |
| C12—C11—H11B | 109.1 | C20—C21—C22 | 113.6 (2) |
| H11A—C11—H11B | 107.9 | C20—C21—H21A | 108.8 |
| C13—C12—C11 | 113.66 (19) | C22—C21—H21A | 108.8 |
| C13—C12—H12A | 108.8 | C20—C21—H21B | 108.8 |
| C11—C12—H12A | 108.8 | C22—C21—H21B | 108.8 |
| C13—C12—H12B | 108.8 | H21A—C21—H21B | 107.7 |
| C11—C12—H12B | 108.8 | C21—C22—H22A | 109.5 |
| H12A—C12—H12B | 107.7 | C21—C22—H22B | 109.5 |
| C12—C13—C14 | 112.95 (19) | H22A—C22—H22B | 109.5 |
| C12—C13—H13A | 109.0 | C21—C22—H22C | 109.5 |
| C14—C13—H13A | 109.0 | H22A—C22—H22C | 109.5 |
| C12—C13—H13B | 109.0 | H22B—C22—H22C | 109.5 |
| C14—C13—H13B | 109.0 | | |
| C8—N1—C1—C2 | 178.1 (2) | C1—N1—C8—C7 | 2.6 (2) |
| C9—N1—C1—C2 | 5.4 (3) | C9—N1—C8—C7 | 175.52 (18) |
| C8—N1—C1—C6 | −1.6 (2) | O1—C7—C8—O2 | −2.9 (4) |
| C9—N1—C1—C6 | −174.36 (18) | C6—C7—C8—O2 | 175.9 (2) |
| C6—C1—C2—C3 | 0.9 (3) | O1—C7—C8—N1 | 178.6 (2) |
| N1—C1—C2—C3 | −178.8 (2) | C6—C7—C8—N1 | −2.7 (2) |
| C1—C2—C3—C4 | −0.4 (3) | C8—N1—C9—C10 | −94.4 (2) |
| C2—C3—C4—C5 | −0.5 (3) | C1—N1—C9—C10 | 77.5 (3) |
| C3—C4—C5—C6 | 0.9 (3) | N1—C9—C10—C11 | 172.23 (18) |
| C4—C5—C6—C1 | −0.4 (3) | C9—C10—C11—C12 | 179.29 (19) |
| C4—C5—C6—C7 | 178.9 (2) | C10—C11—C12—C13 | 175.77 (19) |
| C2—C1—C6—C5 | −0.5 (3) | C11—C12—C13—C14 | 179.72 (19) |
| N1—C1—C6—C5 | 179.22 (19) | C12—C13—C14—C15 | 178.93 (19) |
| C2—C1—C6—C7 | −179.99 (19) | C13—C14—C15—C16 | 179.85 (19) |
| N1—C1—C6—C7 | −0.3 (2) | C14—C15—C16—C17 | 179.82 (19) |
| C5—C6—C7—O1 | 1.0 (4) | C15—C16—C17—C18 | −179.84 (19) |
| C1—C6—C7—O1 | −179.6 (2) | C16—C17—C18—C19 | −179.47 (19) |
| C5—C6—C7—C8 | −177.6 (2) | C17—C18—C19—C20 | −179.98 (19) |
| C1—C6—C7—C8 | 1.8 (2) | C18—C19—C20—C21 | 180.0 (2) |
| C1—N1—C8—O2 | −176.0 (2) | C19—C20—C21—C22 | 179.8 (2) |
| C9—N1—C8—O2 | −3.1 (3) | | |

**Fig. 1**


O1
O2
C7
C8
N1
C6
C5
C9
C11
C10
C2
C13
C12
C4
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C15
C14
C17
C16
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C20
C22