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# (1*H*-1,2,3-Benzotriazol-1-yl)methyl 2,2-dimethylpropanoate

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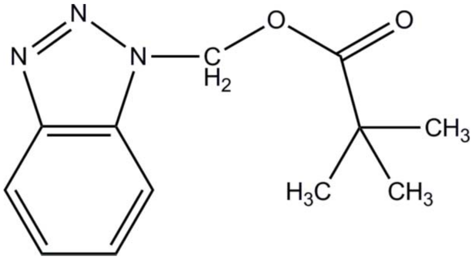
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.043; $wR$ factor = 0.128; data-to-parameter ratio = 10.3.

In the title compound, $C_{12}H_{15}N_3O_2$, the dihedral angle between the mean planes of the benzene and triazole rings is 0.331 (53) °. The side chain of the pivalate unit forms a dihedral angle of 69.04 (12)° with the benzotriazole unit. The ester group and two methyl groups of the pivalate unit are disordered with an occupancy ratio of 0.731 (3):0.269 (3). In the crystal, weak $\pi$–$\pi$ stacking interactions are observed between inversion-related benzene rings [centroid–centroid distance = 3.9040 (1) Å].

## Related literature

For a related structure, see: Li & Chen (2011). For applications of benzotriazole derivatives, see: Wan & Lv (2010). For related coordination compounds, see: Hang & Ye (2008); Xu & Shen (2012).



## Experimental

### Crystal data

$C_{12}H_{15}N_3O_2$
$M_r$ = 233.27
Monoclinic, $P2_1/c$
$a$ = 8.1507 (3) Å
$b$ = 16.7258 (8) Å
$c$ = 9.2967 (4) Å
$\beta$ = 98.354 (3)°
$V$ = 1253.94 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
0.30 × 0.25 × 0.22 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001) $T_{min}$ = 0.975, $T_{max}$ = 0.981
9487 measured reflections
2206 independent reflections
1738 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.128
$S$ = 1.03
2206 reflections
214 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.10 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2123).

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# supporting information

*Acta Cryst.* (2012). E**68**, o1066 [https://doi.org/10.1107/S1600536812010252]

## (1*H*-1,2,3-Benzotriazol-1-yl)methyl 2,2-dimethylpropanoate

**Sen Xu and Yingzhong Shen**

### S1. Comment

Nobenzotriazole derivatives have been extensively studied, not only for their potential application in antibacterial activities (Wan & Lv, 2010), but also for synthesizing benzotriazole coordination complexes (Hang & Ye, 2008). In continuing our work with new benzotriazole coordination complexes (Xu & Shen, 2012), we have synthesized a new N-donor benzotriazole derivative ligand, $C_{12}H_{15}N_3O_2$, Fig. 1 Bond lengths and angles are similar to those in related benzotriazol-1-yl intermediate derivatives (Li & Chen, 2011, Wan & Lv, 2010). The ester group and two methyl groups in the pivalate unit are disordered, In the crystal, weak $\pi$–$\pi$ stacking interactions are observed between the inversion related phenyl rings (centroid-centroid distances = 3.9040 (1)°).

### S2. Experimental

To a 250 ml round flask was added (1*H*-benzo[*d*][1,2,3]triazol-1-yl)methanol(3.73 g, 0.025 mol), methylene chloride(20 mL) and triethylamine(7.0 mL) with magnetic stirring atroom tempertature for 1 h. Pivaloyl chloride(3.32 g, 0.028 mol) was then added to the solution in the ice bath. The mixture was then refluxed for 6 h at 303 K under a nitrogen atmosphere. When the reaction was completed, the solvent was evaporated *in vacuo*, and the residue was washed with distilled water and purified by recrystallization from diethyl ether (Yield: 83.2%). Colorless crystals suitable for X-ray analysis were obtained by slow evaporation from diethyl ether at room temperature.

### S3. Refinement

The H atoms on the $CH_2$ group were located by difference maps and freely refined without constraints. H atoms bonded to the remaining C atoms were included in calculated positions and treated as riding with C–H = 0.93–0.97Å and $U_{iso}$(H)=1.2Ueq(aromatic C) or $U_{iso}$(H) = 1.5Ueq($CH_3$). The ester(–O—CO–) and two methyl groups (C10, C11) in the pivalate unit are disordered over two side positions with site occupation factors 0.731 (3)/0.269 (3). The C—C, C—O distances and angles of the disordered groups were refined without restraints.

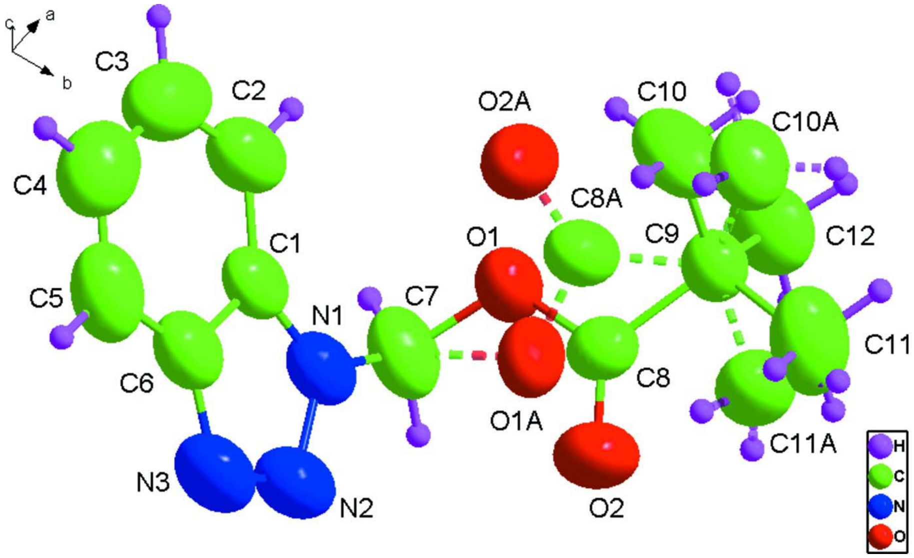

**Figure 1**

The molecular structure of the title compound with 50% probability displacement ellipsoids. Dashed lines indicate disordered ester and methyl groups.

## (1*H*-1,2,3-Benzotriazol-1-yl)methyl 2,2-dimethylpropanoate

### *Crystal data*

$C_{12}H_{15}N_3O_2$
$M_r = 233.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.1507$ (3) Å
$b = 16.7258$ (8) Å
$c = 9.2967$ (4) Å
$\beta = 98.354$ (3)°
$V = 1253.94$ (9) Å$^3$
$Z = 4$
$F(000) = 496$
$D_x = 1.236$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3348 reflections
$\theta = 2.5$–26.7°
$\mu = 0.09$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.30 × 0.25 × 0.22 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.975$, $T_{max} = 0.981$
9487 measured reflections
2206 independent reflections
1738 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -9 \rightarrow 9$
$k = -19 \rightarrow 19$
$l = -11 \rightarrow 10$

### *Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.128$
$S = 1.03$
2206 reflections
214 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 0.1761P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{min} = -0.10$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^{*}=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.240 (12)

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 0.2265 (3) | 0.74088 (14) | 0.5551 (2) | 0.0766 (6) | 0.731 (3) |
| O2 | 0.1680 (2) | 0.82951 (11) | 0.3775 (2) | 0.0968 (7) | 0.731 (3) |
| O1A | 0.1824 (8) | 0.7730 (4) | 0.4914 (9) | 0.0822 (19) | 0.269 (3) |
| O2A | 0.3972 (6) | 0.6944 (3) | 0.5729 (7) | 0.111 (2) | 0.269 (3) |
| N1 | 0.04557 (15) | 0.65313 (9) | 0.40894 (14) | 0.0722 (4) | |
| N2 | −0.05972 (18) | 0.66728 (11) | 0.28420 (19) | 0.0925 (5) | |
| N3 | −0.0594 (2) | 0.60557 (12) | 0.19956 (17) | 0.0958 (5) | |
| C1 | 0.11500 (17) | 0.57919 (10) | 0.40336 (15) | 0.0648 (4) | |
| C2 | 0.2279 (2) | 0.53528 (13) | 0.49892 (19) | 0.0840 (6) | |
| H2 | 0.2739 | 0.5551 | 0.5893 | 0.101* | |
| C3 | 0.2672 (2) | 0.46083 (15) | 0.4516 (3) | 0.1008 (7) | |
| H3 | 0.3428 | 0.4297 | 0.5118 | 0.121* | |
| C4 | 0.1986 (3) | 0.43031 (14) | 0.3178 (3) | 0.1009 (7) | |
| H4 | 0.2283 | 0.3793 | 0.2915 | 0.121* | |
| C5 | 0.0898 (3) | 0.47290 (13) | 0.2249 (2) | 0.0927 (6) | |
| H5 | 0.0446 | 0.4524 | 0.1349 | 0.111* | |
| C6 | 0.04751 (19) | 0.54945 (11) | 0.26945 (18) | 0.0744 (5) | |
| C7 | 0.0640 (2) | 0.71089 (15) | 0.5249 (3) | 0.0871 (6) | |
| H1M | −0.025 (3) | 0.7513 (14) | 0.502 (2) | 0.120 (8)* | |
| H2M | 0.055 (3) | 0.6865 (14) | 0.618 (3) | 0.127 (8)* | |
| C8 | 0.2642 (4) | 0.80275 (16) | 0.4734 (3) | 0.0621 (6) | 0.731 (3) |
| C9 | 0.44199 (18) | 0.83291 (9) | 0.52164 (16) | 0.0637 (4) | |
| C10 | 0.5617 (4) | 0.7648 (2) | 0.5330 (4) | 0.1025 (11) | 0.731 (3) |
| H10A | 0.5324 | 0.7265 | 0.6017 | 0.154* | 0.731 (3) |
| H10B | 0.6717 | 0.7844 | 0.5650 | 0.154* | 0.731 (3) |
| H10C | 0.5581 | 0.7399 | 0.4396 | 0.154* | 0.731 (3) |
| C11 | 0.4801 (6) | 0.8957 (3) | 0.4141 (4) | 0.1158 (13) | 0.731 (3) |
| H11A | 0.4703 | 0.8725 | 0.3187 | 0.174* | 0.731 (3) |
| H11B | 0.5910 | 0.9151 | 0.4419 | 0.174* | 0.731 (3) |

| | | | | | |
|---|---|---|---|---|---|
| H11C | 0.4031 | 0.9392 | 0.4135 | 0.174* | 0.731 (3) |
| C12 | 0.4501 (3) | 0.87363 (13) | 0.6689 (2) | 0.0948 (6) | |
| H12A | 0.3671 | 0.9147 | 0.6633 | 0.142* | |
| H12B | 0.5578 | 0.8970 | 0.6956 | 0.142* | |
| H12C | 0.4304 | 0.8349 | 0.7407 | 0.142* | |
| C8A | 0.3453 (9) | 0.7596 (5) | 0.5306 (7) | 0.0724 (18) | 0.269 (3) |
| C10A | 0.6271 (11) | 0.8008 (6) | 0.4959 (10) | 0.093 (3) | 0.269 (3) |
| H10D | 0.6735 | 0.7684 | 0.5770 | 0.139* | 0.269 (3) |
| H10E | 0.6983 | 0.8458 | 0.4873 | 0.139* | 0.269 (3) |
| H10F | 0.6172 | 0.7696 | 0.4085 | 0.139* | 0.269 (3) |
| C11A | 0.3845 (15) | 0.8843 (7) | 0.3900 (12) | 0.111 (3) | 0.269 (3) |
| H11D | 0.3597 | 0.8509 | 0.3057 | 0.166* | 0.269 (3) |
| H11E | 0.4705 | 0.9214 | 0.3756 | 0.166* | 0.269 (3) |
| H11F | 0.2868 | 0.9132 | 0.4052 | 0.166* | 0.269 (3) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0696 (14) | 0.0778 (14) | 0.0794 (12) | −0.0172 (11) | 0.0009 (9) | 0.0118 (10) |
| O2 | 0.0858 (12) | 0.0929 (13) | 0.1025 (14) | 0.0056 (10) | −0.0178 (10) | 0.0215 (11) |
| O1A | 0.062 (4) | 0.068 (4) | 0.118 (5) | −0.009 (3) | 0.017 (3) | 0.009 (3) |
| O2A | 0.076 (3) | 0.093 (4) | 0.156 (5) | −0.011 (3) | −0.008 (3) | 0.044 (4) |
| N1 | 0.0554 (7) | 0.0852 (10) | 0.0737 (8) | −0.0143 (7) | 0.0016 (6) | 0.0047 (7) |
| N2 | 0.0710 (9) | 0.1006 (12) | 0.0981 (12) | −0.0067 (8) | −0.0137 (8) | 0.0126 (10) |
| N3 | 0.0864 (10) | 0.1078 (13) | 0.0844 (10) | −0.0175 (9) | −0.0168 (8) | 0.0037 (10) |
| C1 | 0.0488 (7) | 0.0823 (11) | 0.0636 (9) | −0.0170 (7) | 0.0091 (6) | 0.0083 (8) |
| C2 | 0.0680 (10) | 0.1065 (15) | 0.0754 (10) | −0.0131 (10) | 0.0034 (8) | 0.0167 (10) |
| C3 | 0.0809 (12) | 0.1038 (16) | 0.1190 (17) | 0.0079 (11) | 0.0189 (12) | 0.0314 (14) |
| C4 | 0.0994 (15) | 0.0939 (15) | 0.1166 (17) | −0.0059 (12) | 0.0396 (13) | 0.0078 (14) |
| C5 | 0.0960 (13) | 0.1002 (15) | 0.0861 (12) | −0.0315 (12) | 0.0270 (11) | −0.0105 (12) |
| C6 | 0.0626 (9) | 0.0894 (12) | 0.0709 (10) | −0.0198 (8) | 0.0083 (7) | 0.0050 (9) |
| C7 | 0.0694 (11) | 0.0980 (14) | 0.0957 (14) | −0.0240 (11) | 0.0185 (9) | −0.0136 (12) |
| C8 | 0.0670 (15) | 0.0573 (14) | 0.0606 (13) | 0.0068 (15) | 0.0046 (13) | 0.0034 (12) |
| C9 | 0.0650 (9) | 0.0635 (9) | 0.0618 (9) | −0.0068 (7) | 0.0064 (6) | −0.0023 (7) |
| C10 | 0.0652 (17) | 0.106 (3) | 0.134 (3) | 0.0108 (16) | 0.0070 (16) | −0.040 (2) |
| C11 | 0.133 (3) | 0.126 (3) | 0.091 (2) | −0.052 (3) | 0.025 (2) | 0.0067 (19) |
| C12 | 0.1017 (14) | 0.1004 (14) | 0.0820 (12) | −0.0055 (11) | 0.0122 (10) | −0.0232 (11) |
| C8A | 0.060 (4) | 0.082 (5) | 0.074 (4) | −0.001 (4) | 0.003 (3) | 0.017 (4) |
| C10A | 0.079 (5) | 0.093 (6) | 0.109 (6) | −0.010 (4) | 0.024 (4) | −0.003 (5) |
| C11A | 0.107 (7) | 0.100 (7) | 0.114 (7) | −0.021 (6) | −0.022 (6) | 0.040 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C8 | 1.345 (4) | C8—C9 | 1.539 (4) |
| O1—C7 | 1.406 (3) | C9—C8A | 1.466 (8) |
| O2—C8 | 1.186 (3) | C9—C10 | 1.493 (3) |
| O1A—C8A | 1.344 (10) | C9—C11 | 1.512 (4) |
| O1A—C7 | 1.481 (8) | C9—C11A | 1.513 (9) |

| | | | |
|---|---|---|---|
| O2A—C8A | 1.215 (10) | C9—C12 | 1.522 (2) |
| N1—N2 | 1.3594 (19) | C9—C10A | 1.651 (9) |
| N1—C1 | 1.364 (2) | C10—H10A | 0.9600 |
| N1—C7 | 1.439 (2) | C10—H10B | 0.9600 |
| N2—N3 | 1.298 (2) | C10—H10C | 0.9600 |
| N3—C6 | 1.378 (2) | C11—H11A | 0.9600 |
| C1—C6 | 1.379 (2) | C11—H11B | 0.9600 |
| C1—C2 | 1.392 (2) | C11—H11C | 0.9600 |
| C2—C3 | 1.374 (3) | C12—H12A | 0.9600 |
| C2—H2 | 0.9300 | C12—H12B | 0.9600 |
| C3—C4 | 1.385 (3) | C12—H12C | 0.9600 |
| C3—H3 | 0.9300 | C10A—H10D | 0.9600 |
| C4—C5 | 1.348 (3) | C10A—H10E | 0.9600 |
| C4—H4 | 0.9300 | C10A—H10F | 0.9600 |
| C5—C6 | 1.404 (3) | C11A—H11D | 0.9600 |
| C5—H5 | 0.9300 | C11A—H11E | 0.9600 |
| C7—H1M | 0.99 (2) | C11A—H11F | 0.9600 |
| C7—H2M | 0.97 (2) | | |

| | | | |
|---|---|---|---|
| C8—O1—C7 | 116.6 (3) | C11—C9—C11A | 30.7 (3) |
| C8A—O1A—C7 | 118.3 (8) | C8A—C9—C12 | 106.0 (3) |
| N2—N1—C1 | 109.84 (14) | C10—C9—C12 | 109.57 (19) |
| N2—N1—C7 | 120.41 (17) | C11—C9—C12 | 107.3 (2) |
| C1—N1—C7 | 129.67 (16) | C11A—C9—C12 | 116.2 (5) |
| N3—N2—N1 | 108.78 (15) | C8A—C9—C8 | 41.5 (3) |
| N2—N3—C6 | 108.23 (14) | C10—C9—C8 | 110.42 (19) |
| N1—C1—C6 | 104.36 (14) | C11—C9—C8 | 108.1 (2) |
| N1—C1—C2 | 133.91 (16) | C11A—C9—C8 | 77.4 (4) |
| C6—C1—C2 | 121.73 (18) | C12—C9—C8 | 108.94 (14) |
| C3—C2—C1 | 115.92 (18) | C8A—C9—C10A | 104.2 (4) |
| C3—C2—H2 | 122.0 | C10—C9—C10A | 33.0 (3) |
| C1—C2—H2 | 122.0 | C11—C9—C10A | 81.4 (4) |
| C2—C3—C4 | 122.6 (2) | C11A—C9—C10A | 104.5 (6) |
| C2—C3—H3 | 118.7 | C12—C9—C10A | 110.8 (4) |
| C4—C3—H3 | 118.7 | C8—C9—C10A | 133.9 (4) |
| C5—C4—C3 | 121.5 (2) | C9—C10—H10A | 109.5 |
| C5—C4—H4 | 119.2 | C9—C10—H10B | 109.5 |
| C3—C4—H4 | 119.2 | C9—C10—H10C | 109.5 |
| C4—C5—C6 | 117.38 (19) | C9—C11—H11A | 109.5 |
| C4—C5—H5 | 121.3 | C9—C11—H11B | 109.5 |
| C6—C5—H5 | 121.3 | C9—C11—H11C | 109.5 |
| N3—C6—C1 | 108.78 (17) | C9—C12—H12A | 109.5 |
| N3—C6—C5 | 130.39 (18) | C9—C12—H12B | 109.5 |
| C1—C6—C5 | 120.82 (18) | H12A—C12—H12B | 109.5 |
| O1—C7—N1 | 112.46 (17) | C9—C12—H12C | 109.5 |
| O1—C7—O1A | 33.7 (2) | H12A—C12—H12C | 109.5 |
| N1—C7—O1A | 108.3 (3) | H12B—C12—H12C | 109.5 |
| O1—C7—H1M | 115.9 (14) | O2A—C8A—O1A | 121.4 (8) |

| | | | |
|---|---|---|---|
| N1—C7—H1M | 107.8 (13) | O2A—C8A—C9 | 127.2 (6) |
| O1A—C7—H1M | 87.4 (14) | O1A—C8A—C9 | 111.3 (7) |
| O1—C7—H2M | 99.3 (14) | C9—C10A—H10D | 109.5 |
| N1—C7—H2M | 111.8 (14) | C9—C10A—H10E | 109.5 |
| O1A—C7—H2M | 128.2 (14) | H10D—C10A—H10E | 109.5 |
| H1M—C7—H2M | 109.4 (18) | C9—C10A—H10F | 109.5 |
| O2—C8—O1 | 122.3 (4) | H10D—C10A—H10F | 109.5 |
| O2—C8—C9 | 125.9 (3) | H10E—C10A—H10F | 109.5 |
| O1—C8—C9 | 111.7 (2) | C9—C11A—H11D | 109.5 |
| C8A—C9—C10 | 73.1 (3) | C9—C11A—H11E | 109.5 |
| C8A—C9—C11 | 141.4 (3) | H11D—C11A—H11E | 109.5 |
| C10—C9—C11 | 112.4 (3) | C9—C11A—H11F | 109.5 |
| C8A—C9—C11A | 114.5 (5) | H11D—C11A—H11F | 109.5 |
| C10—C9—C11A | 127.8 (6) | H11E—C11A—H11F | 109.5 |

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| C1—N1—N2—N3 | −0.27 (18) | C7—O1—C8—O2 | −2.4 (4) |
| C7—N1—N2—N3 | −177.51 (15) | C7—O1—C8—C9 | 177.12 (17) |
| N1—N2—N3—C6 | 0.17 (19) | O2—C8—C9—C8A | −157.5 (5) |
| N2—N1—C1—C6 | 0.25 (16) | O1—C8—C9—C8A | 23.0 (4) |
| C7—N1—C1—C6 | 177.16 (14) | O2—C8—C9—C10 | −130.2 (3) |
| N2—N1—C1—C2 | −179.74 (16) | O1—C8—C9—C10 | 50.3 (3) |
| C7—N1—C1—C2 | −2.8 (3) | O2—C8—C9—C11 | −6.9 (3) |
| N1—C1—C2—C3 | 179.88 (16) | O1—C8—C9—C11 | 173.7 (3) |
| C6—C1—C2—C3 | −0.1 (2) | O2—C8—C9—C11A | −4.3 (6) |
| C1—C2—C3—C4 | −0.5 (3) | O1—C8—C9—C11A | 176.3 (6) |
| C2—C3—C4—C5 | 0.8 (3) | O2—C8—C9—C12 | 109.4 (2) |
| C3—C4—C5—C6 | −0.5 (3) | O1—C8—C9—C12 | −70.0 (2) |
| N2—N3—C6—C1 | −0.02 (19) | O2—C8—C9—C10A | −102.3 (5) |
| N2—N3—C6—C5 | 179.30 (17) | O1—C8—C9—C10A | 78.2 (5) |
| N1—C1—C6—N3 | −0.14 (16) | C7—O1A—C8A—O2A | 10.7 (10) |
| C2—C1—C6—N3 | 179.85 (14) | C7—O1A—C8A—C9 | −166.6 (4) |
| N1—C1—C6—C5 | −179.54 (13) | C10—C9—C8A—O2A | 17.8 (7) |
| C2—C1—C6—C5 | 0.5 (2) | C11—C9—C8A—O2A | 122.8 (7) |
| C4—C5—C6—N3 | −179.41 (17) | C11A—C9—C8A—O2A | 142.3 (9) |
| C4—C5—C6—C1 | −0.2 (2) | C12—C9—C8A—O2A | −88.2 (7) |
| C8—O1—C7—N1 | 85.2 (3) | C8—C9—C8A—O2A | 171.1 (10) |
| C8—O1—C7—O1A | −4.4 (4) | C10A—C9—C8A—O2A | 28.7 (9) |
| N2—N1—C7—O1 | −118.0 (2) | C10—C9—C8A—O1A | −165.1 (6) |
| C1—N1—C7—O1 | 65.3 (3) | C11—C9—C8A—O1A | −60.2 (8) |
| N2—N1—C7—O1A | −82.3 (3) | C11A—C9—C8A—O1A | −40.7 (9) |
| C1—N1—C7—O1A | 101.1 (4) | C12—C9—C8A—O1A | 88.8 (6) |
| C8A—O1A—C7—O1 | 17.8 (4) | C8—C9—C8A—O1A | −11.8 (4) |
| C8A—O1A—C7—N1 | −85.5 (6) | C10A—C9—C8A—O1A | −154.2 (6) |