organic compounds

3,4,5-Trihydroxy-N'-(1-methyl-1H-indol-2-yl)methylidene]benzohydrazide

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The structure of the title compound, C 17 H 15 N 3 O 4 , displays intermolecular O-H-N and O-H-O hydrogen bonding between adjacent molecules. Intramolecular O-H-H and O hydrogen bonds also occur. The molecule is essentially planar with a deviation of 0.090 (1) Å from the best plane running through the connected ring systems.

Related literature

For related compounds see: Khaledi et al. (2008 a,b, 2009).

Experimental

Crystal data

- C 17 H 15 N 3 O 4
- M r = 325.32
- Monoclinic, P 2 1 / n
- a = 9.0839 (2) Å
- b = 13.1684 (3) Å
- c = 12.4414 (3) Å
- β = 104.2740 (10)°
- V = 1442.30 (6) Å³
- Z = 4
- Mo Kα radiation
- μ = 0.11 mm⁻¹
- T = 100 K
- 0.49 × 0.16 × 0.09 mm
Data collection

- Bruker APEXII CCD area-detector diffractometer
- Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $T_{\text{min}} = 0.948$, $T_{\text{max}} = 0.991$
- 10177 measured reflections
- 4070 independent reflections
- 3153 reflections with $I > 2\sigma(I)$
- $R_{\text{int}} = 0.019$

Refinement

- $R[F^2 > 2\sigma(F^2)] = 0.044$
- $wR(F^2) = 0.127$
- $S = 0.99$
- 4070 reflections
- 221 parameters
- H-atom parameters constrained
- $\Delta \rho_{\text{max}} = 0.63$ e $\text{Å}^{-3}$
- $\Delta \rho_{\text{min}} = -0.26$ e $\text{Å}^{-3}$

Table 1

<table>
<thead>
<tr>
<th>D-H, $\alpha$</th>
<th>D-H</th>
<th>H-A</th>
<th>D, $\alpha$</th>
<th>D-H, $\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>O2-H2O, , O4$^i$</td>
<td>0.84</td>
<td>1.80</td>
<td>2.6119 (14)</td>
<td>164</td>
</tr>
<tr>
<td>O1-H1O, , N2$^i$</td>
<td>0.84</td>
<td>2.06</td>
<td>2.7759 (15)</td>
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</tr>
<tr>
<td>O3-H3O, , O2$^ii$</td>
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<td>2.12</td>
<td>2.8469 (14)</td>
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<tr>
<td>O1-H1O, , O2</td>
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<td>2.51</td>
<td>2.8570 (14)</td>
<td>106</td>
</tr>
<tr>
<td>O3-H3O, , O2</td>
<td>0.84</td>
<td>2.31</td>
<td>2.7560 (14)</td>
<td>113</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) $x$, $\frac{1}{2}$, $y$, $-\frac{1}{2}$, $z$; (ii) $-x+2$, $-y$, $-z$.

Data collection: APEX2 (Bruker, 2007); cell refinement: APEX2; data reduction: SAINT (Bruker, 2007); 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, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2532).

Acknowledgements
The authors thank the University of Malaya for funding this study (FRGS grant No. FP009/2008 C).

References


