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Tris(2-cyanoethyl)amine

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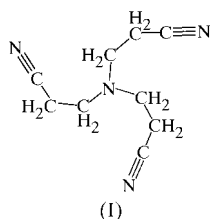
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In the title compound, $N(\text{CH}_2\text{CH}_2\text{CN})_3$, (I), the three cyanoethyl groups adopt a conformation with the CN groups



oriented in the same direction, suggesting the compound may behave as a potential tripodal ligand.

Experimental

The title compound was recrystallized from ethanol.

Crystal data

$\text{C}_9\text{H}_{12}\text{N}_4$
 $M_r = 176.23$
 Orthorhombic, $Pna2_1$
 $a = 8.1341$ (12) Å
 $b = 13.4171$ (19) Å
 $c = 9.2291$ (14) Å
 $V = 1007.2$ (3) Å³
 $Z = 4$
 $D_x = 1.162$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 474 reflections
 $\theta = 3.67$ – 13.14°
 $\mu = 0.075$ mm⁻¹
 $T = 293$ (2) K
 Block, colourless
 $0.25 \times 0.20 \times 0.05$ mm

Data collection

Bruker Smart 1K CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (Blessing, 1995)
 $T_{\min} = 0.981$, $T_{\max} = 0.996$
 5674 measured reflections
 2178 independent reflections

1691 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\text{max}} = 27.06^\circ$
 $h = -7 \rightarrow 10$
 $k = -13 \rightarrow 17$
 $l = -11 \rightarrow 11$
 Intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.081$
 $S = 0.995$
 2178 reflections
 118 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.10$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.09$ e Å⁻³
 Absolute structure: Flack (1983)
 Flack parameter = 0 (2); 1005
 Friedel-related reflections

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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