

(*R,R*)-1-Acetyl-1'-(2,4,6-trinitrophenyl)-2,2'-bipyrrolidine

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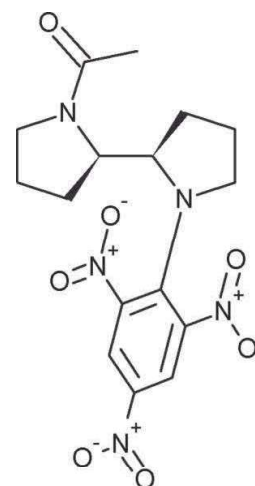
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.043; wR factor = 0.090; data-to-parameter ratio = 7.2.

The structure of the title molecule, $\text{C}_{16}\text{H}_{19}\text{N}_5\text{O}_7$, is mainly determined by the steric effect of a bulky 2,4,6-trinitrophenyl group attached to the N atom of a pyrrolidine ring. Both pyrrolidine rings adopt an envelope conformation, with one of the methylene C atoms as the flap in each case, and the N—C—C—N torsion angle along the bond connecting the two pyrrolidine rings is -174.9 (2)°. The benzene ring of the 2,3,5-trinitrophenyl substituent is deformed and the r.m.s. deviation of its six atoms from the best plane is 0.026 Å. The N atoms of the two nitro groups in the *ortho* positions deviate from the best plane of the benzene ring by -0.033 (5) and 0.385 (5) Å. These groups, as well as the pyrrolidine ring, are twisted relative to the aromatic ring in the same direction, their best planes forming dihedral angles of 30.2 (2), 64.8 (1) and 46.6 (2)°, respectively, with the ring. An intramolecular C—H...O hydrogen bond occurs. In the crystal, there is a short [O...C = 3.019 (4) Å] contact between a nitro O atom and a C atom of the benzene ring bearing the nitro group and a C—H...O interaction between a methyl H atom and another nitro O atom.

Related literature

For crystal structures of related 1-amino-2,4,6-trinitrobenzenes, see: Butcher *et al.* (1992); Baggio *et al.* (1997).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{19}\text{N}_5\text{O}_7$	$V = 1788.63$ (19) Å ³
$M_r = 393.36$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.1989$ (5) Å	$\mu = 0.12$ mm ⁻¹
$b = 10.4442$ (6) Å	$T = 293$ K
$c = 20.8877$ (13) Å	$0.20 \times 0.20 \times 0.15$ mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer	7678 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2012)	1818 independent reflections
$T_{\min} = 0.990$, $T_{\max} = 1.000$	1477 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	254 parameters
$wR(F^2) = 0.090$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\max} = 0.14$ e Å ⁻³
1818 reflections	$\Delta\rho_{\min} = -0.16$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C2}-\text{H2}\cdots\text{O1}$	0.98	2.18	2.891 (4)	129
$\text{C18}-\text{H18C}\cdots\text{O2}^i$	0.96	2.51	3.454 (5)	168

Symmetry code: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5033).

References

- Agilent (2012). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
 Baggio, R., Remedi, M. V., Garland, M. T. & Bujan, E. I. (1997). *J. Chem. Crystallogr.* **27**, 499–505.