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(7-Isopropyl-1,4a-dimethyl-1,2,3,4,4a,-9,10,10a-octahydrophenanthren-1-yl)-methanaminium 4-toluenesulfonate

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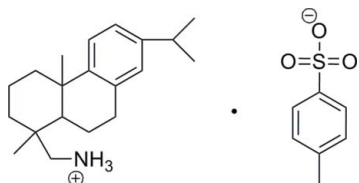
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in main residue; R factor = 0.046; wR factor = 0.140; data-to-parameter ratio = 16.5.

In the title compound, $\text{C}_{20}\text{H}_{32}\text{N}^+\cdot\text{C}_7\text{H}_7\text{O}_3\text{S}^-$, the configurations of the two chiral centers observed in the protonated cation are consistent with previous reports. In the crystal structure, weak intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link ions into chains which develop along the a axis. The isopropyl group and four CH groups of the attached benzene ring are disordered approximately equally over two positions.

Related literature

For related literature, see: Gottstein & Cheney (1965); Rao *et al.* (2006); Tao (1993).



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{32}\text{N}^+\cdot\text{C}_7\text{H}_7\text{O}_3\text{S}^-$ $M_r = 457.65$ Orthorhombic, $P2_12_12_1$ $a = 5.9954$ (2) Å $b = 11.7039$ (5) Å $c = 37.0381$ (13) Å $V = 2598.95$ (17) Å³ $Z = 4$ Mo $K\alpha$ radiation
 $\mu = 0.15$ mm⁻¹ $T = 296$ (2) K
 $0.40 \times 0.30 \times 0.30$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Absorption correction: multi-scan

(SADABS; Bruker, 2000)

 $T_{\min} = 0.942$, $T_{\max} = 0.956$ 22386 measured reflections
5925 independent reflections
4346 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.045$ $wR(F^2) = 0.139$ $S = 1.05$

5925 reflections

360 parameters

204 restraints

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.22$ e Å⁻³ $\Delta\rho_{\min} = -0.35$ e Å⁻³

Absolute structure: Flack (1983),

2489 Friedel pairs

Flack parameter: 0.03 (8)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1C}\cdots\text{O1}$	0.89	2.06	2.835 (3)	145
$\text{N1}-\text{H1D}\cdots\text{O3}^{\text{i}}$	0.89	1.84	2.722 (3)	173
$\text{N1}-\text{H1E}\cdots\text{O1}^{\text{ii}}$	0.89	1.95	2.772 (3)	152

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

Data collection: SMART (Bruker, 2002); cell refinement: SAINT-Plus (Bruker, 2003); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEPIII (Burnett & Johnson, 1996), ORTEP3 (Farrugia, 1997) and XP in SHELXTL; software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2336).

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