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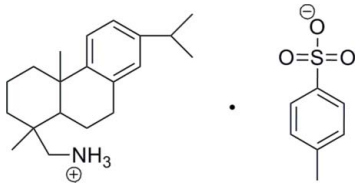
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.046; wR factor = 0.140; data-to-parameter ratio = 16.5.

In the title compound, $C_{20}H_{32}N^+\cdot C_7H_7O_3S^-$, the configurations of the two chiral centers observed in the protonated cation are consistent with previous reports. In the crystal structure, weak intermolecular N—H···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

$C_{20}H_{32}N^+\cdot C_7H_7O_3S^-$
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) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 296 (2) K
0.40 × 0.30 × 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_{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···A	D—H	H···A	D···A	D—H···A
N1—H1C···O1	0.89	2.06	2.835 (3)	145
N1—H1D···O3^{i}	0.89	1.84	2.722 (3)	173
N1—H1E···O1^{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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