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1-(*p*-Anisyl)-2-carboxyethanaminium *p*-toluenesulfonate

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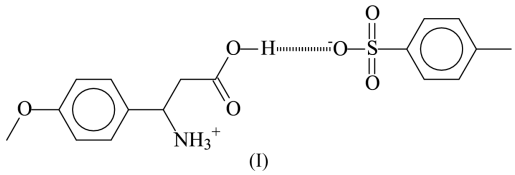
The cation and anion in the title compound, $C_{10}H_{14}NO_3^+\cdot C_7H_7O_3S^-$, (I), are linked by a short carboxylic acid–sulfonate O···O hydrogen bond. Adjacent ion pairs are linked by hydrogen bonds involving the ammonium unit, giving rise to tightly held chains that run along the *b* axis of the monoclinic unit cell.



(I)

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.058
wR factor = 0.166
Data-to-parameter ratio = 13.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Experimental

The title compound, (I), was the unintended product of the reaction between *p*-anisyl-β-alanine and *p*-toluenesulfonyl chloride in an attempt to place the sulfonyl on the amino portion of the β-alanine molecule. The two reagents, in mmol scale, were reacted in stoichiometric proportions in ethanol for several hours. The reaction was then quenched by the addition of hydrochloric acid. The white compound that separated was recrystallized from ethanol (m.p. >573 K).

Crystal data

$C_{10}H_{14}NO_3^+\cdot C_7H_7O_3S^-$
M_r = 367.41
Monoclinic, $P2_1/c$
a = 8.095 (2) Å
b = 6.448 (2) Å
c = 34.733 (3) Å
β = 96.43 (2)°
V = 1801.7 (6) Å^3
Z = 4
D_x = 1.354 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 8.3–11.3°
μ = 0.21 mm^{-1}
T = 298 (2) K
Block, colorless
0.3 × 0.3 × 0.2 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: empirical *via* ψ scan (North *et al.*, 1968)
T_{min} = 0.505, T_{max} = 0.954
3417 measured reflections
3174 independent reflections
2139 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°
h = −9 → 0
k = −7 → 0
l = −41 → 41
3 standard reflections
frequency: 60 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.166
S = 1.05
3174 reflections
244 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0861P)^2 + 0.6702P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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Table 1
Selected geometric parameters (Å, °).

S1—O2	1.435 (3)	C4—C5	1.375 (7)
S1—O1	1.447 (3)	C4—C7	1.518 (6)
S1—O3	1.447 (3)	C5—C6	1.373 (6)
S1—C1	1.756 (3)	C8—C9	1.489 (4)
O4—C8	1.196 (4)	C9—C10	1.522 (5)
O5—C8	1.327 (4)	C10—C12	1.503 (4)
O6—C15	1.366 (4)	C12—C17	1.376 (5)
O6—C18	1.415 (6)	C12—C13	1.387 (5)
N1—C10	1.505 (4)	C13—C14	1.374 (5)
C1—C6	1.374 (5)	C14—C15	1.383 (6)
C1—C2	1.381 (5)	C15—C16	1.370 (5)
C2—C3	1.378 (5)	C16—C17	1.383 (5)
C3—C4	1.378 (6)		
O1—S1—O2	114.7 (2)	O4—C8—O5	122.5 (3)
O1—S1—O3	110.4 (2)	O4—C8—C9	125.1 (3)
O2—S1—O3	112.8 (2)	O5—C8—C9	112.4 (3)
O1—S1—C1	105.8 (2)	C8—C9—C10	113.1 (3)
O2—S1—C1	105.7 (2)	C12—C10—N1	109.4 (3)
O3—S1—C1	106.9 (2)	C12—C10—C9	114.6 (3)
C15—O6—C18	117.7 (4)	N1—C10—C9	109.1 (3)
C2—C1—C6	119.9 (3)	C10—C12—C13	122.8 (3)
C6—C1—S1	120.8 (3)	C10—C12—C17	119.3 (3)
C2—C1—S1	119.3 (3)	C13—C12—C17	117.9 (3)
C1—C2—C3	119.4 (4)	C12—C13—C14	120.6 (4)
C2—C3—C4	121.3 (4)	C13—C14—C15	120.7 (3)
C3—C4—C5	118.1 (4)	O6—C15—C16	125.4 (4)
C3—C4—C7	120.8 (5)	O6—C15—C14	115.4 (3)
C5—C4—C7	121.1 (5)	C14—C15—C16	119.2 (3)
C4—C5—C6	121.6 (4)	C15—C16—C17	119.7 (4)
C1—C6—C5	119.7 (4)	C12—C17—C16	121.8 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*o*···O1	0.85 (1)	1.81 (1)	2.653 (3)	169 (5)
N1—H2*n*···O2^{i}	0.85 (1)	1.90 (1)	2.736 (4)	167 (4)
N1—H1*n*···O3^{ii}	0.86 (1)	2.02 (2)	2.811 (5)	152 (4)
N1—H3*n*···O3^{iii}	0.86 (1)	2.12 (2)	2.903 (4)	152 (3)

Symmetry codes: (i) $1-x, -y, 1-z$; (ii) $1-x, 1-y, 1-z$; (iii) $x, y-1, z$.

The aryl and alkyl H atoms were placed at calculated positions (aryl C—H = 0.93 Å and alkyl C—H = 0.96 Å) and were included in the refinement in the riding-model approximation; $U_{iso}(H) = 1.2U_{eq}(C)$. The methyl groups were allowed to rotate about their local threefold axes. The carboxylic acid and ammonium H atoms were located and refined using a distance restraint (O—H = N—H = 0.85 (1) Å).

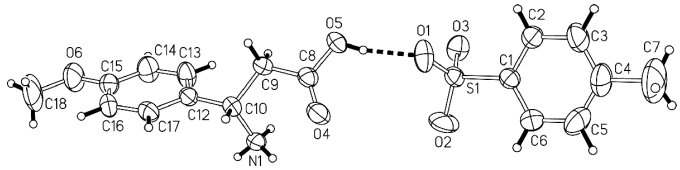

Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. The dashed line indicates the hydrogen bond

Data collection: *CAD*-4/*PC* (Kretschmar, 1994); cell refinement: *CAD*-4 *VAX/PC* Fortran System (Enraf–Nonius, 1988); data reduction: *XCAD*4 (Harms, 1997) in *WinGX* (Farrugia, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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