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(*E*)-4-{[(3-Propyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-4-yl)imino]methyl}-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olate

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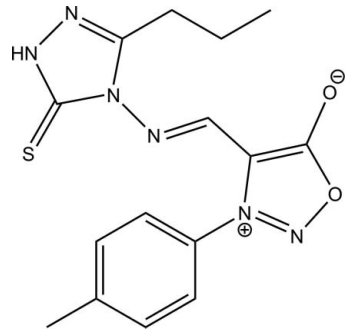
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.039; wR factor = 0.123; data-to-parameter ratio = 20.6.

The title compound, $C_{15}H_{16}N_6O_2S$, exists in a *trans* configuration with respect to the acyclic N=C bond. The 1,2,3-oxadiazol-3-ium ring makes dihedral angles of 10.59 (8) and 73.94 (8)°, respectively, with the 1,2,4-triazole and benzene rings. The molecular structure is stabilized by an intramolecular C—H···S hydrogen bond, which generates an S(6) ring motif. In the crystal, molecules are linked into inversion dimers by pairs of intermolecular N—H···S hydrogen bonds, generating eight-membered $R_2^2(8)$ ring motifs. The dimers are further connected by C—H···O hydrogen bonds, forming a sheet parallel to the *bc* plane. The ethyl group is disordered over two sets of sites with occupancies of 0.744 (7) and 0.256 (7).

Related literature

For general background to and applications of sydnone derivatives, see: Baker *et al.* (1949); Hedge *et al.* (2008); Rai *et al.* (2008); Kalluraya *et al.* (2002). For standard bond-length data, see: Allen *et al.* (1987). For graph-set notation, see: Bernstein *et al.* (1995). For a related structure, see: Fun *et al.* (2011).



Experimental

Crystal data

$C_{15}H_{16}N_6O_2S$
M_r = 344.40
Monoclinic, $P2_1/c$
a = 13.4220 (11) Å
b = 6.2411 (5) Å
c = 21.1374 (16) Å
β = 104.575 (2)°
V = 1713.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 K
0.51 × 0.17 × 0.08 mm

Data collection

Bruker SMART APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.865, T_{max} = 0.983
18912 measured reflections
5003 independent reflections
3637 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.123
S = 1.04
5003 reflections
243 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H1*N5*···S1^{i}	0.857 (18)	2.440 (18)	3.2933 (13)	174.3 (16)
C1—H1*A*···O2^{ii}	0.93	2.48	3.346 (2)	154
C9—H9*A*···S1	0.93	2.42	3.1845 (13)	139

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2776).

‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5525-2009.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Baker, W., Ollis, W. D. & Poole, V. D. (1949). *J. Chem. Soc.* pp. 307–314.

Bernstein, J., Davis, R. E., Shimoni, L. & Chamg, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Fun, H.-K., Quah, C. K., Nithinchandra & Kalluraya, B. (2011). *Acta Cryst.* E**67**, o1005–o1006.

Hedge, J. C., Girisha, K. S., Adhikari, A. & Kalluraya, B. (2008). *Eur. J. Med. Chem.* **43**, 2831–2834.

Kalluraya, B., Rahiman, A. & David, B. (2002). *Indian J. Chem. Sect. B*, **41**, 1712–1717.

Rai, N. S., Kalluraya, B., Lingappa, B., Shenoy, S. & Puranic, V. G. (2008). *Eur. J. Med. Chem.* **43**, 1715–1720.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.