Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,1,1-Trifluoro-4-(thiophen-2-yl)-4-[(2-{[4,4,4-trifluoro-3-oxo-1-(thiophen-2-yl)but-1-en-1-yl]amino}ethyl)amino]but-3-en-2-one

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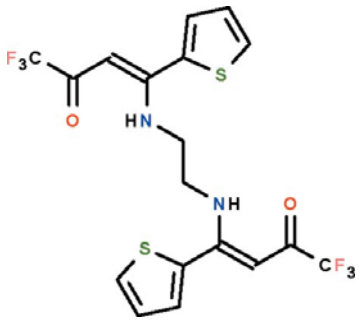
Received 11 September 2011; accepted 11 September 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.046; wR factor = 0.122; data-to-parameter ratio = 14.5.

The asymmetric unit of the diamine compound, $C_{18}H_{14}F_3N_2O_2S_2$, consists of two molecules; the C=C double bond has a Z configuration in the $C_4H_3S-C=C-C(=O)-C$ segment. The $-NH-CH_2-CH_2-NH$ chain adopts a twisted U-shape. The amino group is an intramolecular hydrogen-bond donor to the carbonyl group; the intramolecular hydrogen bond generates a six-membered ring. In both molecules, the thienyl rings are disordered over two positions; the occupancies of the major components are 0.817 (4) and 0.778 (4) in one molecule and 0.960 (4) and 0.665 (4) in the other. One of the trifluoromethyl groups is disordered over two positions with the major component having 0.637 (8) occupancy.

Related literature

For the synthesis, see: Wang & Tong (1995). For related structures, see: Bresciani-Pahor *et al.* (1979); Haider *et al.* (1981).



Experimental

Crystal data

$C_{18}H_{14}F_6N_2O_2S_2$
M_r = 468.43
Orthorhombic, $Pna2_1$
a = 20.4520 (4) Å
b = 12.5201 (2) Å
c = 15.8328 (2) Å
V = 4054.16 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.906, T_{max} = 0.936
40183 measured reflections
9198 independent reflections
8265 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
S = 1.05
9198 reflections
633 parameters
242 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Absolute structure: Flack (1983), 4340 Friedel pairs
Flack parameter: 0.01 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n···O1	0.88 (1)	2.03 (3)	2.741 (3)	138 (3)
N2—H2n···O2	0.88 (1)	2.01 (3)	2.726 (3)	138 (3)
N3—H3n···O3	0.88 (1)	1.93 (3)	2.668 (3)	140 (3)
N4—H4n···O4	0.87 (1)	1.96 (3)	2.677 (3)	139 (3)

Data collection: *CrysAlis PRO* (Agilent, 2010); 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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5326).