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(*E*)-2-Methyl-5-(thiophen-2-ylmethylidene)cyclopentan-1-one

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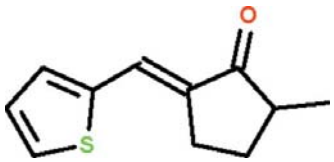
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.041; wR factor = 0.104; data-to-parameter ratio = 17.5.

The exocyclic C=C double-bond in the title compound, $C_{11}H_{12}OS$, has an *E* configuration. The methyl-bearing C atom in the cyclopentane ring is disordered over two positions with a site-occupation factor of 0.899 (8) for the major occupied site.

Related literature

For the synthesis of 2-(2-thienylidene)cyclopentanone, see: Austin *et al.* (2007); Tsukerman *et al.* (1964).



Experimental

Crystal data

$C_{11}H_{12}OS$
M_r = 192.27
Monoclinic, $P2_1/c$
a = 12.0667 (5) Å
b = 11.0576 (4) Å
c = 7.3003 (3) Å
β = 100.469 (4)°
V = 957.85 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 100 K
0.25 × 0.15 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.931, T_{max} = 0.971
4842 measured reflections
2131 independent reflections
1817 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.104
S = 0.99
2131 reflections
122 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5619).

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