Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1′-(4-Iodobenzyl)spiro[isobenzofuran-1(3*H*),4′-piperidine]

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Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.003 Å
R factor = 0.024
wR factor = 0.059
Data-to-parameter ratio = 21.1

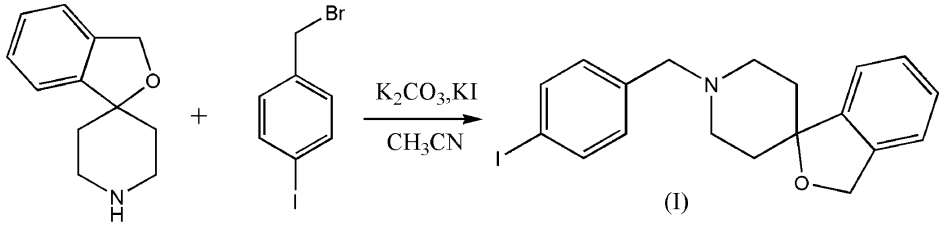
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{19}H_{20}INO$, the central piperidine ring adopts a chair conformation.

Received 20 March 2007
Accepted 31 March 2007

Comment

Among many different structural classes of sigma-1 receptor ligands, the spiropiperidines offer the best potential sigma-1 receptor affinity and selectivity towards the sigma-2 receptor and other brain receptors (Maier & Wuensch, 2002*a*,*b*). In this context, the crystal structures are very important for understanding the interaction between the ligand and the sigma receptor.



(I)

The molecular structure of the title compound, (I), is shown in Fig. 1. The fused benzene ring makes a dihedral angle of 20.1 (1)° with the plane composed of the three atoms O1, C8 and C1, the five-membered ring being an envelope with O1 at the flap position. The piperidine ring adopts a chair conformation.

Experimental

Compound (I) was synthesized according to the literature method of Kubota *et al.* (1998) (see scheme). Single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from a mixture of petroleum ether and diethyl ether (*v*:*v* 5:1) over a period of 1 d.

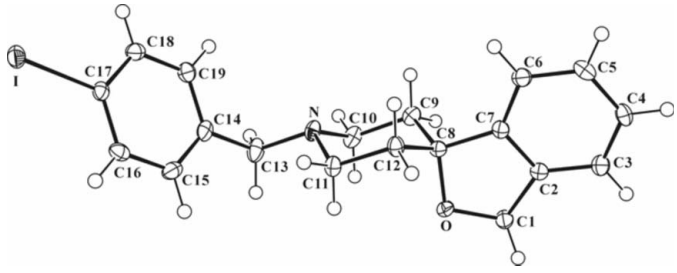


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

Crystal data

$C_{19}H_{20}INO$
$M_r = 405.26$
Monoclinic, $P2_1/c$
$a = 10.1099\ (6)$ Å
$b = 11.8733\ (6)$ Å
$c = 14.262\ (1)$ Å
$\beta = 105.722\ (3)^\circ$
$V = 1647.98\ (17)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.95$ mm^{-1}
$T = 113\ (2)$ K
$0.24 \times 0.20 \times 0.18$ mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min} = 0.653$, $T_{max} = 0.721$
15887 measured reflections
4225 independent reflections
3599 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.059$
$S = 1.05$
4225 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.81$ e Å^{-3}

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aromatic H and 0.99 Å for methylene H, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

This work was supported by the National Natural Science Foundation of China (grant No. NSFC 20501004).

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