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N-[2-(2-Methoxyphenyl)benzylidene]-*tert*-butylamine *N*-oxide

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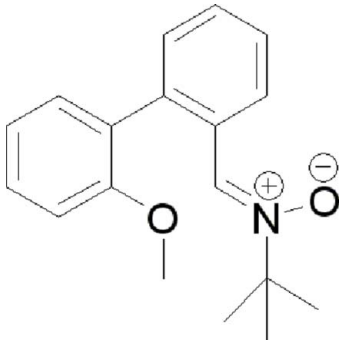
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.058; data-to-parameter ratio = 10.4.

In the molecule of the title compound, $C_{18}H_{21}NO_2$, the two benzene rings are oriented at a dihedral angle of 58.19 (3)°. Intramolecular C—H···O hydrogen bonds result in the formation of one six- and one five-membered ring, which adopt twist and envelope conformations, respectively. In the crystal structure, C—H···O hydrogen bonds link the molecules.

Related literature

For general background, see: Hamburger & McCay (1989); Jotti *et al.* (1992); Murphy *et al.* (2003); Green *et al.* (2003); Durand *et al.* (2007); Hay *et al.* (2005). For related literature, see: Fevig *et al.* (1996).



Experimental

Crystal data

$C_{18}H_{21}NO_2$
M_r = 283.37
Monoclinic, $P2_1$
a = 10.2526 (15) Å
b = 8.5576 (13) Å
c = 10.3333 (16) Å
β = 115.742 (3)°
V = 816.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 (1) K
0.30 × 0.28 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.968, T_{max} = 0.993
7869 measured reflections
1981 independent reflections
967 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.058
S = 1.00
1981 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 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
C3—H3···O1	0.93	2.26	2.806 (3)	117
C17—H171···O1	0.96	2.41	2.791 (3)	104
C18—H181···O1^{i}	0.96	2.50	3.280 (3)	139

Symmetry code: (i) $-x+2, y-\frac{1}{2}, -z+2$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004) and Larson (1970); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2462).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Durand, G., Poeggeler, B., Boker, J., Raynal, S., Polidori, A., Pappolla, M. A., Hardeland, R. & Pucci, B. (2007). *J. Med. Chem.* **50**, 3976–3979.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Fevig, T. L., Bowen, S. M., Janowick, D. A., Jones, B. K., Munson, H. R., Ohlweiler, D. F. & Thomas, G. E. (1996). *J. Med. Chem.* **39**, 4988–4996.
Green, A. R., Ashwood, T., Odergren, T. & Jackson, D. M. (2003). *Pharm. Ther.* **100**, 195–214.
Hamburger, S. A. & McCay, P. B. (1989). *Circ. Shock*, **29**, 329–334.
Hay, A., Burkitt, M. J., Jones, C. M. & Hartley, R. C. (2005). *Arch. Biochem. Biophys.* **435**, 336–346.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Jotti, A., Paracchini, L., Perletti, G. & Piccinini, F. (1992). *Pharmcol. Res.* **26**, 143–150.
Larson, A. C. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, pp. 291–294. Copenhagen: Munksgaard.
Murphy, M. P., Echtay, K. S., Blaikie, F. H., Asin-Gayuela, J., Cocheme, H. M., Green, K., Buckingam, J. A., Taylor, E. R., Hurrell, F., Hughes, G., Miwa, S., Cooper, C. E., Svitunenko, D. A., Smith, R. A. J. & Brand, M. D. (2003). *J. Biol. Chem.* **278**, 48534–48545.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2004). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.