Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-[(*tert*-Butyldimethylsilyl)oxy]-6-methoxy-7-methyl-5-(oxiran-2-ylmethyl)-2-benzofuran-3(1*H*)-one

Magdalena Malachowska-Ugarte, Grzegorz Cholewinski,* Jaroslaw Chojnacki and Krystyna Dzierzbicka

Chemical Faculty, Gdansk University of Technology, Narutowicza 11/12, Gdansk PL-80233, Poland
Correspondence e-mail: gch@chem.pg.gda.pl

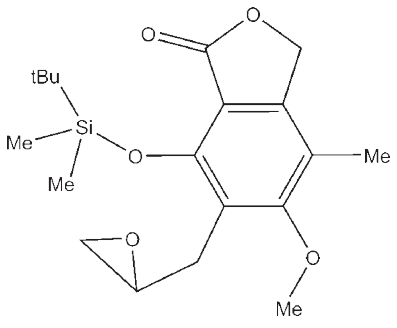
Received 5 October 2011; accepted 17 November 2011

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.045; wR factor = 0.123; data-to-parameter ratio = 14.1.

The title compound, $C_{19}H_{28}O_5Si$, was obtained in the reaction of 1,3-dihydro-4-[(*tert*-butyldimethylsilyl)oxy]-6-methoxy-7-methyl-3-oxo-5-(prop-2-enyl)isobenzofuran with *meta*-chloroperbenzoic acid. This reaction is one of the stages of the total synthesis of mycophenolic acid, which we attempted to modify. The title compound forms crystals with only weak intermolecular interactions. The strongest stacking interaction is found between the benzene and furan rings of inversion-related molecules with a distance of 3.8773 (13) Å between the ring centroids.

Related literature

For structures of related oxiranes, see: Langer & Becker (1993); Berthalon *et al.* (1999). For the preparation of the title compound, see: Patterson (1995); Plé *et al.* (1997). For the properties of epoxides, see: Padwa & Murphree (2006). For a description of the Cambridge Structural Database, see Allen (2002).



Experimental

Crystal data

$C_{19}H_{28}O_5Si$
M_r = 364.5
Monoclinic, $P2_1/c$
a = 7.5682 (3) Å
b = 12.2488 (4) Å
c = 20.6905 (8) Å
β = 93.990 (4)°
V = 1913.39 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 120 K
0.55 × 0.44 × 0.35 mm

Data collection

Agilent Xcalibur diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
T_{min} = 0.938, T_{max} = 0.954
6727 measured reflections
3430 independent reflections
2858 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.123
S = 1.09
3430 reflections
243 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *publCIF* (Westrip, 2010), *PLATON* (Spek, 2009), *WinGX* (Farrugia, 1999) and *Mercury* (Macrae *et al.*, 2006).

We would like to thank the National Centre for Research and Development (Poland) for financial support (grant No. LIDER/07/581L-2/10/NCBiR/2011)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2029).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Berthalon, S., Motta-Viola, L., Regnouf-de-Vains, J.-B., Lamartine, R., Lecocq, S. & Perrin, M. (1999). *Eur. J. Org. Chem.* pp. 2269–2274.
Clark, R. C. & Reid, J. S. (1995). *Acta Cryst.* A**51**, 887–897.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Langer, V. & Becker, H.-D. (1993). *Z. Kristallogr.* **207**, 153–155.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Padwa, A. & Murphree, S. S. (2006). *ARKIVOC*, **iii**, 6–33.
Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
Patterson, J. W. (1995). *J. Org. Chem.* **60**, 4542–4548.
Plé, P. A., Hamon, A. & Jones, G. (1997). *Tetrahedron*, **53**, 3395–3400.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.