

# Xanthurenic acid, O,O'-bis(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester

Other names: Xanthurenic acid, tert-BDMS  
Xanthurenic acid, O,O'-(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester  
Xanthurenic acid, 3tbdms derivative

**Inchi:** InChI=1S/C28H49NO4Si3/c1-26(2,3)34(10,11)31-22-18-16-17-20-23(32-35(12,13)27(4,5

**InchiKey:** IRJIRIHKMGRQPY-UHFFFAOYSA-N

**Formula:** C28H49NO4Si3

**SMILES:** CC(C)(C)[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C(C)(C)C)c2cccc(O[Si](C)(C)C(C)(C)C)c2n1

**Mol. weight [g/mol]:** 547.95

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	9.165		Crippen Method
rinpola	3004.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333761&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpola:** Non-polar retention indices

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