

# Baicalein, TMS

**Inchi:** InChI=1S/C24H34O5Si3/c1-30(2,3)27-21-16-20-22(18(25)15-19(26-20)17-13-11-10-12-14)31-23-24  
**InchiKey:** CEHSKUAHPOYRLD-UHFFFAOYSA-N  
**Formula:** C<sub>24</sub>H<sub>34</sub>O<sub>5</sub>Si<sub>3</sub>  
**SMILES:** C[Si](C)(C)Oc1cc2oc(-c3ccccc3)cc(=O)c2c(O[Si](C)(C)C)c1O[Si](C)(C)C  
**Mol. weight [g/mol]:** 486.78

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.06		Crippen Method
logp	7.101		Crippen Method
rinpol	2861.30		NIST Webbook
rinpol	2904.90		NIST Webbook
rinpol	2861.30		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=R746&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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<https://www.chemeo.com/cid/117-008-3/Baicalein-TMS.pdf>

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