

3-Methyl-2-butenyl-3-acetyloxycaffeate, TMS

Inchi: InChI=1S/C22H34O6Si2/c1-16(2)12-13-25-21(24)11-10-18-14-19(26-17(3)23)22(28-30(7)
InchiKey: UZYCIVYKDKQUMK-ZHACJKMWSA-N
Formula: C22H34O6Si2
SMILES: CC(=O)Oc1cc(C=CC(=O)OCC=C(C)C)cc(O[Si](C)(C)C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 450.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	5.562		Crippen Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R403004&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/33-916-8/3-Methyl-2-butenyl-3-acetyloxycaffeate-TMS.pdf>

Generated by Cheméo on 2024-04-26 17:23:41.186643204 +0000 UTC m=+16441470.107220516.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.