

Copalol, TMS

Inchi: InChI=1S/C23H42OSi/c1-18(14-17-24-25(6,7)8)10-12-20-19(2)11-13-21-22(3,4)15-9-16-
InchiKey: DQWJLUBHVBNA CB-MEECRAKQSA-N
Formula: C₂₃H₄₂OSi
SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1CCC(C)=CCO[Si](C)(C)C
Mol. weight [g/mol]: 362.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	7.363		Crippen Method
rinpol	2302.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585314&Units=SI>

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.chemeo.com/cid/64-723-8/Copalol-TMS.pdf>

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