

ent-Kaurenol TMS

Inchi: InChI=1S/C23H40OSi/c1-17-14-23-13-10-19-21(2,16-24-25(4,5)6)11-7-12-22(19,3)20(23)
InchiKey: ROUGQYHITZRPPQ-PZNBRSVSA-N
Formula: C23H40OSi
SMILES: C=C1CC23CCC4C(C)(CO[Si](C)(C)C)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]: 360.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	6.807		Crippen Method
rinpol	2329.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R396015&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/12-266-3/ent-Kaurenol-TMS.pdf>

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