

Physcion-9-anthrone, TMS

Inchi: InChI=1S/C25H38O4Si3/c1-17-12-18-14-19-15-20(26-2)16-22(28-31(6,7)8)24(19)25(29-
InchiKey: RVUZQCVGYSFFNY-UHFFFAOYSA-N
Formula: C25H38O4Si3
SMILES: COc1cc(O[Si](C)(C)C)c2c(O[Si](C)(C)C)c3c(O[Si](C)(C)C)cc(C)cc3cc2c1
Mol. weight [g/mol]: 486.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	7.951		Crippen Method
rinpol	2652.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158284&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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/58-949-5/Physcion-9-anthrone-TMS.pdf>

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