Radicicol, tris(trimethylsilyl) ether

Other names: Zeranol, 3tms derivative
Inchi: InChI=1S/C27H50O5Si3/c1-21-15-14-18-23(30-33(2,3)4)17-13-11-12-16-22-19-24(31-34
InchiKey: WAEKBNXYNALRQQ-UHFFFAOYSA-N
Formula: C27H50O5Si3
SMILES: CC1CCCC(O[Si](C)(C)C)CCCCCc2cc(O[Si](C)(C)C)cc(O[Si](C)(C)C)c2C(=O)O1
Mol. weight [g/mol]: 538.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	8.166		Crippen Method
rinpol	2822.20		NIST Webbook
rinpol	2822.20		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333479&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/86-432-7/Radicicol-tris-trimethylsilyl-ether.pdf
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