Salsolinol, TMS

Inchi: InChI=1S/C17H31NO2Si2/c1-13-15-12-16(19-2)17(20-22(6,7)8)11-14(15)9-10-18(13)21(
InchiKey: KYDKUJLXKIKZRW-ZDUSSCGKSA-N
Formula: C17H31NO2Si2
SMILES: COc1cc2c(cc1O[Si](C)(C)C)CCN([Si](C)(C)C)C2C
Mol. weight [g/mol]: 337.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.43		Crippen Method
logp	4.663		Crippen Method
rinpol	1950.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R305074&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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