Benzyl 4-[(trimethylsilyl)oxy]benzoate

Other names: Benzyl (E)-p-coumarate, mono-TMS
Inchi: InChI=1S/C17H20O3Si/c1-21(2,3)20-16-11-9-15(10-12-16)17(18)19-13-14-7-5-4-6-8-14/
InchiKey: HVEKDTUCYABGMC-UHFFFAOYSA-N
Formula: C17H20O3Si
SMILES: C[Si](C)(C)Oc1ccc(C(=O)OCc2ccccc2)cc1
Mol. weight [g/mol]: 300.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	4.257		Crippen Method
rinpol	2476.00		NIST Webbook
rinpol	2476.00		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=U408178&Units=SI

Legend

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