Dihydroxyacetone, (O-pentafluorobenzyl)oxime, bis(trimethylsilyl) ether

Other names: Dihydroxyacetone, O-pentafluorobenzyloxime, TMS

Inchi: InChI=1S/C26H24F5NO3Si2/c1-26(2,3)24-7-10(8-25-27(4,5)6)22-23-9-11-12(17)14(19)1

InchiKey: USWYPJDAMDAWJD-UHFFFAOYSA-N

Formula: C16H24F5NO3Si2

SMILES: C[Si](C)(C)OCC(CO[Si](C)(C)C)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 429.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	4.958		Crippen Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U157026&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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