2-Phenylethanamine DMPFPS

Inchi: InChI=1S/C16H16F5NSi/c1-23(2,22-9-8-10-6-4-3-5-7-10)16-14(20)12(18)11(17)13(19)15

InchiKey: PASGPSQKXAMQCH-UHFFFAOYSA-N

Formula: C16H16F5NSi

SMILES: C[Si](C)(NCCc1ccccc1)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 345.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.60		Crippen Method
logp	3.626		Crippen Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R102404&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