Phenylethanolamine, N-methyl, N-DTFMB-TMS

Inchi: InChI=1S/C21H23F6NO2Si/c1-28(13-18(30-31(2,3)4)14-8-6-5-7-9-14)19(29)15-10-16(20
InchiKey: CKJMVNRUFSZQOO-UHFFFAOYSA-N
Formula: C21H23F6NO2Si
SMILES: CN(CC(O[Si](C)(C)C)c1ccccc1)C(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 463.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	6.389		Crippen Method
rinpol	1966.00		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=R165034&Units=SI

Legend

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