Phenylethanolamine, N-DTFMB-TMS

Inchi: InChI=1S/C20H21F6NO2Si/c1-30(2,3)29-17(13-7-5-4-6-8-13)12-27-18(28)14-9-15(19(21
InchiKey: LKXNJZGLXIYALL-UHFFFAOYSA-N
Formula: C20H21F6NO2Si
SMILES: C[Si](C)(C)OC(CNC(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1)c1ccccc1
Mol. weight [g/mol]: 449.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	6.047		Crippen Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R165029&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