4-Methylbenzoic acid DMPFPS

Inchi: InChI=1S/C16H13F5O2Si/c1-8-4-6-9(7-5-8)16(22)23-24(2,3)15-13(20)11(18)10(17)12(19

InchiKey: SFMPOMPQTREENX-UHFFFAOYSA-N

Formula: C16H13F5O2Si

SMILES: Cc1ccc(C(=O)O[Si](C)(C)c2c(F)c(F)c(F)c(F)c2F)cc1

Mol. weight [g/mol]: 360.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.91		Crippen Method
logp	3.960		Crippen Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R102464&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices