4-Bromophenol DMPFPS

Inchi: InChI=1S/C14H10BrF5OSi/c1-22(2,21-8-5-3-7(15)4-6-8)14-12(19)10(17)9(16)11(18)13(1
InchiKey: CVMWIBMDZPUBRF-UHFFFAOYSA-N
Formula: C14H10BrF5OSi
SMILES: C[Si](C)(Oc1ccc(Br)cc1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 397.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.48		Crippen Method
logp	4.636		Crippen Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		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=R102444&Units=SI

Legend

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