

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: SFMPOMPQTREEENX-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
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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/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-063-1/4-Methylbenzoic-acid-DMPFPS.pdf>

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