Silane, trimethyl[5-methyl-2-(1-methylethyl)phenoxy]-

Other names: Thymol-TMS

2-Isopropyl-5-methylphenol, TMS

Thymol, tms derivative

Inchi: InChl=1S/C13H22OSi/c1-10(2)12-8-7-11(3)9-13(12)14-15(4,5)6/h7-10H,1-6H3

InchiKey: UTGMDFONUNJYQP-UHFFFAOYSA-N

Formula: C13H22OSi

SMILES: Cc1ccc(C(C)C)c(O[Si](C)(C)C)c1

Mol. weight [g/mol]: 222.40 CAS: 55012-80-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	4.332		Crippen Method
rinpol	1301.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1310.00		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=C55012801&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/llogp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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