

Eugenol TMS

Inchi:	InChI=1S/C13H20O2Si/c1-6-7-11-8-9-12(13(10-11)14-2)15-16(3,4)5/h6,8-10H,1,7H2,2-5
InchiKey:	YUXGSLPZJFDWGG-UHFFFAOYSA-N
Formula:	C13H20O2Si
SMILES:	C=CCc1ccc(O[Si](C)(C)C)c(OC)c1
Mol. weight [g/mol]:	236.38
CAS:	4515-52-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.67		Crippen Method
logp	3.637		Crippen Method
rinsol	1472.80		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4515520&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/122-099-7/Eugenol-TMS.pdf>

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