

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.67		Crippen Method
logp	3.637		Crippen Method
rinpol	1472.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1472.00		NIST Webbook

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=U71757&Units=SI>

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/125-102-9/Eugenol-TMS.pdf>

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