

Chavicol TMS

Inchi: InChI=1S/C12H18OSi/c1-5-6-11-7-9-12(10-8-11)13-14(2,3)4/h5,7-10H,1,6H2,2-4H3
InchiKey: LXMWEQRAJHXKBM-UHFFFAOYSA-N
Formula: C12H18OSi
SMILES: C=CCc1ccc(O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 206.36
CAS: 218618-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	3.629		Crippen Method
rinpol	1320.60		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C218618792&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/85-667-8/Chavicol-TMS.pdf>

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