

4-(7-Ethyl-3-methyl-5-propenyl-2,3-dihydro-benzo

TES

InChIKey:

InChI=1S/C27H38O3Si/c1-8-13-20-16-21(9-2)27-23(17-20)19(6)26(29-27)22-14-15-24(2

LGRGTCOLAFFZOF-MDWZMJQESA-N

Formula:

C27H38O3Si

SMILES:

CC=Cc1cc(CC)c2c(c1)C(C)C(c1ccc(O[Si](CC)(CC)CC)c(OC)c1)O2

Mol. weight [g/mol]:

438.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.75		Crippen Method
logp	7.912		Crippen Method
rinpol	3060.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R294409&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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