

Silane, (1,1-dimethylethyl)dimethyl[(6,6,9-trimethyl-3-pen

Other names:

Cannabinol tert-butyldimethylsilyl ether
tert-Butyl(dimethyl)[(6,6,9-trimethyl-3-pentyl-6H-benzo[c]chromen-1-yl)oxy]silane
Cannabinol, tbdms derivative

Inchi: InChI=1S/C27H40O2Si/c1-10-11-12-13-20-17-23-25(24(18-20)29-30(8,9)26(3,4)5)21-16

InchiKey: XNSPKWBHHSYZSF-UHFFFAOYSA-N

Formula: C27H40O2Si

SMILES: CCCCCc1cc2c(c(O[Si](C)(C)C(C)(C)C)c1)-c1cc(C)ccc1C(C)(C)O2

Mol. weight [g/mol]: 424.69

CAS: 61595-80-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	8.406		Crippen Method
rinpol	2699.50		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C61595800&Units=SI>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/11-078-3/Silane-1-1-dimethylethyl-dimethyl-6-6-9-trimethyl-3-pentyl-6H-dibenzo-b-d-py>

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