

Cardanol C19:1 (TMS)

Inchi: InChI=1S/C28H50OSi/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-27-24-22-2
InchiKey: NJFQNMYYFOHKQGU-KHPPLWFESA-N
Formula: C28H50OSi
SMILES: CCCCCC=CCCCCCCCCCCCc1ccc(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 430.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.25		Crippen Method
logp	9.870		Crippen Method
rinpol	2882.20		NIST Webbook
rinpol	2882.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U414072&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/72-814-8/Cardanol-C19-1-TMS.pdf>

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