d3-morphine, di-TMS

Inchi: InChI=1S/C23H35NO3Si2/c1-24-13-12-23-16-9-11-19(27-29(5,6)7)22(23)25-21-18(26-28
InchiKey: WGFFZYSWLVJOLB-JFXVRRSHSA-N
Formula: C23H32D3NO3Si2
SMILES: CN1CCC23c4c5ccc(O[Si](C)(C)C)c4OC2C(O[Si](C)(C)C)C=CC3C1C5
Mol. weight [g/mol]: 432.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	4.565		Crippen Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R501252&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