4-Androsten-3-.beta.,17-.beta.-diol, TMS

Inchi: InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey: APMJYCGLEHJTKS-CESWCLKUSA-N
Formula: C25H46O2Si2
SMILES: C[C@]12CC[C@H](O[Si](C)(C)C)C=C1CCC1C2CC[C@@]2(C)C1CC[C@@H]2O[Si](C)(
Mol. weight [g/mol]: 434.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Cheméo Relay (1.0)
logp	7.389		Crippen Method
tf	384.51	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R384646
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
tf: Normal melting (fusion) point