5-«beta»-Cholestan-3-one, oxime, TMS # 2

Inchi: InChI=1S/C30H55NOSi/c1-21(2)10-9-11-22(3)26-14-15-27-25-13-12-23-20-24(31-32-33(
InchiKey: VSEPXMZPXCXVEF-RZIUYZJTSA-N
Formula: C30H55NOSi
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CC(=NO[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 473.85

Physical Properties

Property code	Value	Unit	Source
hvap	118.49	kJ/mol	Cheméo Relay (1.0)
log10ws	-8.37		Cheméo Relay (1.0)
logp	9.315		Crippen Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook
tb	701.58	K	Cheméo Relay (1.0)
tf	373.29	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R215733&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point