Dihydrocodeine tms derivative

Other names:	6-«alpha»-Hydrocodol, TMS
	Dihydrocodeine O-TMS
	Dihydrocodeine TMS
Inchi:	InChI=1S/C21H31NO3Si/c1-22-11-10-21-14-7-9-17(25-26(3,4)5)20(21)24-19-16(23-2)8-(
InchiKey:	GZSGQWPBDZITGJ-UHFFFAOYSA-N
Formula:	C21H31NO3Si
SMILES:	COc1ccc2c3c1OC1C(O[Si](C)(C)C)CCC4C(C2)N(C)CCC341
Mol. weight [g/mol]:	373.57

Physical Properties

Property code	Value	Unit	Source
ie	7.84	eV	Cheméo Relay (1.0)
log10ws	-2.80		Cheméo Relay (1.0)
logp	3.584		Crippen Method
tf	376.98	K	Cheméo Relay (1.0)

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U137060&Units=SI

Legend

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