

Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-6-((5«alpha»,6«alpha»)-

Other names: Codeine, TMS derivative
Codeine, O-trimethylsilyl-

Codeine, mono-TMS

Codeine O-TMS

Codeine, TMS

O-(Trimethylsilyl)codeine

Hydrocodone O-TMS

Hydrocodone, mono-TMS

Hydrocodone TMS

Inchi: InChI=1S/C21H29NO3Si/c1-22-11-10-21-14-7-9-17(25-26(3,4)5)20(21)24-19-16(23-2)8-

InchiKey: RXSDDUCBUIPWHI-UHFFFAOYSA-N

Formula: C21H29NO3Si

SMILES: COc1ccc2c3c1OC1C(O[Si](C)(C)C)C=CC4C(C2)N(C)CCC341

Mol. weight [g/mol]: 371.55

CAS: 74367-14-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	3.360		Crippen Method
rinpol	2490.00		NIST Webbook
rinpol	2479.30		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367149&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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