INDICINE PERTRIMETHYLSILYL ETHER

Other names: Indicine pertrimethylsilyl ether
Echinatine, triTMS
Inchi: InChI=1S/C24H49NO5Si3/c1-18(2)24(30-33(10,11)12,19(3)28-31(4,5)6)23(26)27-17-20-
InchiKey: BNOZTCHGOQKVFR-UHFFFAOYSA-N
Formula: C24H49NO5Si3
SMILES: CC(C)C(O[Si](C)(C)C)(C(=O)OCC1=CCN2CCC(O[Si](C)(C)C)C12)C(C)O[Si](C)(C)C
Mol. weight [g/mol]: 515.92

Physical Properties

Property code	Value	Unit	Source
logp	5.250		Crippen Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71307227&Units=SI
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

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/124-668-3/INDICINE-PERTRIMETHYLSILYL-ETHER.pdf
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