

adhulupone

Inchi: InChI=1S/C24H46O4Si3/c1-14-18(4)21(25)20-22(26-29(5,6)7)19(16-15-17(2)3)23(27-30)
InchiKey: QOTXXWKURYZLJS-UHFFFAOYSA-N
Formula: C24H46O4Si3
SMILES: CCC(C)C(=O)C1=C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CC=C(C)C)=C1O[Si](C)(C)C
Mol. weight [g/mol]: 482.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	7.403		Crippen Method
rinpol	2124.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2124.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R384215&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-519-1/adhulupone.pdf>

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