1-Heptanol, O-TBDMS

Inchi: InChI=1S/C13H30OSi/c1-7-8-9-10-11-12-14-15(5,6)13(2,3)4/h7-12H2,1-6H3
InchiKey: SSKLQKJXKUELBH-UHFFFAOYSA-N
Formula: C13H30OSi
SMILES: CCCCCCCO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 230.46
CAS: 115306-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	4.979		Crippen Method
rinpol	1293.00		NIST Webbook
rinpol	1293.40		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1293.40		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C115306893&Units=SI

Legend

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

ripol: Polar retention indices