

2-Ketocaproic acid, diTBDMMS

Inchi: InChI=1S/C18H38O3Si2/c1-12-13-14-15(20-22(8,9)17(2,3)4)16(19)21-23(10,11)18(5,6)7
InchiKey: WKFOEZMZZHXNDF-PFONDFGASA-N
Formula: C18H38O3Si2
SMILES: CCCC=C(O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 358.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	6.241		Crippen Method
rinpol	1768.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U332346&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/42-153-5/2-Ketocaproic-acid-diTBDMMS.pdf>

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