

2-Ketocaproic acid, MO TBDMS # 1

Inchi: InChI=1S/C13H27NO3Si/c1-8-9-10-11(14-16-5)12(15)17-18(6,7)13(2,3)4/h8-10H2,1-7H3
InchiKey: BTYPTKZEDRJFFP-UHFFFAOYSA-N
Formula: C13H27NO3Si
SMILES: CCCCC(=NOC)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 273.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	3.727		Crippen Method
rinpol	1440.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R563156&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/70-857-3/2-Ketocaproic-acid-MO-TBDMS-1.pdf>

Generated by Cheméo on 2024-04-29 05:54:41.644575985 +0000 UTC m=+16659330.565153301.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.