

.alpha.-Ketooctanoic acid, MO TBDMS # 1

Inchi: InChI=1S/C15H31NO3Si/c1-8-9-10-11-12-13(16-18-5)14(17)19-20(6,7)15(2,3)4/h8-12H2
InchiKey: PCQUTROEACGARX-UHFFFAOYSA-N
Formula: C15H31NO3Si
SMILES: CCCCCC(=NOC)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 301.50

Physical Properties

Property code	Value	Unit	Source
logp	4.508		Crippen Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R562722&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/33-437-0/alpha-Ketooctanoic-acid-MO-TBDMS-1.pdf>

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