3-methyl-2-ketobutyric acid TMS

Other names: 2-Ketoisovaleric acid, TMS # 1
Inchi: InChI=1S/C8H16O3Si/c1-6(2)7(9)8(10)11-12(3,4)5/h6H,1-5H3
InchiKey: VFKKKSSJRGFPIS-UHFFFAOYSA-N
Formula: C8H16O3Si
SMILES: CC(C)C(=O)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 188.30

Physical Properties

Property code	Value	Unit	Source
logp	1.590		Crippen Method
rinpol	1048.00		NIST Webbook
rinpol	1048.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367707&Units=SI

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices