2-ketovaleric acid TMS

Other names:	2-Ketovaleric acid, TMS # 1
	2-Ketovaleric acid, TMS ester
	2-Oxopentanoic acid, tms derivative
	«alpha»-Ketovaleric acid, TMS
Inchi:	InChI=1S/C8H16O3Si/c1-5-6-7(9)8(10)11-12(2,3)4/h5-6H2,1-4H3
InchiKey:	KXURKMKWKFOXLN-UHFFFAOYSA-N
Formula:	C8H16O3Si
SMILES:	CCCC(=O)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	188.30

Physical Properties

Property code	Value	Unit	Source
logp	1.734		Crippen Method
tb	453.07	K	Cheméo Relay (1.0)

Sources

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=C74367694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
tb:	Normal Boiling Point Temperature

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