

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

Latest version available from:

<https://www.chemeo.com/cid/97-061-7/3-methyl-2-ketobutyric-acid-TMS.pdf>

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