

Succinylacetone, TMS, # 2

Other names:	Succinylacetone, TMS, # 1 Succinylacetone, TMS
Inchi:	InChI=1S/C13H26O4Si2/c1-11(14)10-12(16-18(2,3)4)8-9-13(15)17-19(5,6)7/h10H,8-9H2
InchiKey:	JTZWNADIMKBHCO-BENRWUELSA-N
Formula:	C13H26O4Si2
SMILES:	CC(=O)C=C(CCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	302.51

Physical Properties

Property code	Value	Unit	Source
log10ws	1.06		Crippen Method
logp	3.469		Crippen Method
rinpol	1644.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R401602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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.chemeo.com/cid/44-798-8/Succinylacetone-TMS-2.pdf>

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