

2-Ketoadipic acid mo-tbdms

Other names:	2-Ketohexanedioic acid mo-tbdms
Inchi:	InChI=1S/C19H39NO5Si2/c1-18(2,3)26(8,9)24-16(21)14-12-13-15(20-23-7)17(22)25-27(
InchiKey:	QZUJNZWYYAUSBD-UHFFFAOYSA-N
Formula:	C19H39NO5Si2
SMILES:	CON=C(CCCC(=O)O[Si](C)(C)C(C)(C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	417.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	5.256		Crippen Method
rinsol	2103.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332312&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/81-987-7/2-Ketoadipic-acid-mo-tbdms.pdf>

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