

2-Ketoadipic acid ditbdms

Other names:	2-Ketohexanedioic acid ditbdms 2-Ketoadipic acid, 2tbdms derivative
Inchi:	InChI=1S/C18H36O5Si2/c1-17(2,3)24(7,8)22-15(20)13-11-12-14(19)16(21)23-25(9,10)18
InchiKey:	FQYCCNNEBKBSIY-UHFFFAOYSA-N
Formula:	C18H36O5Si2
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)CCCC(=O)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	388.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.46		Crippen Method
logp	4.823		Crippen Method
rinpol	2054.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332330&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/33-093-2/2-Ketoadipic-acid-ditbdms.pdf>

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