2-Ketoadipic acid, oxime, tri-TMS

Other names:	2-Oxohexanedioic acid, oxime, tris-TMS
	2-Ketoadipic acid, oxime, TMS
	oximated 2-keto-adipic acid, triTMS
	2-Ketoadipic acid, oxime, tris-TMS
	Hexanedioic acid, «alpha»-keto oxime, (trimethylsilyl)-
Inchi:	InChI=1S/C15H33NO5Si3/c1-22(2,3)19-14(17)12-10-11-13(16-21-24(7,8)9)15(18)20-23(
InchiKey:	HUDNSTCQNYJCQY-UHFFFAOYSA-N
Formula:	C15H33NO5Si3
SMILES:	C[Si](C)(C)ON=C(CCCC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	391.68
CAS:	59-78-9

Physical Properties

Property code	Value	Unit	Source
log10ws	2.78		Crippen Method
logp	4.120		Crippen Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1732.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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