

# 2-Ketoadipic acid, oxime, tri-TMS

<b>Other names:</b>	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)-
<b>Inchi:</b>	InChI=1S/C15H33NO5Si3/c1-22(2,3)19-14(17)12-10-11-13(16-21-24(7,8)9)15(18)20-23(
<b>InchiKey:</b>	HUDNSTCQNYJCQY-UHFFFAOYSA-N
<b>Formula:</b>	C15H33NO5Si3
<b>SMILES:</b>	C[Si](C)(C)ON=C(CCCC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	391.68
<b>CAS:</b>	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

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

# 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.cheméo.com/cid/53-559-3/2-Ketoadipic-acid-oxime-tri-TMS.pdf>

Generated by Cheméo on 2024-05-11 18:37:57.167817351 +0000 UTC m=+17741926.088394664.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.