

# Aconitic acid, tri-TMS

<b>Other names:</b>	Aconitic acid, tris-trimethylsilyl ester Aconitic acid, TMS ACONITIC ACID 3TMS Aconitic acid, tris-TMS
<b>Inchi:</b>	InChI=1S/C15H30O6Si3/c1-22(2,3)19-13(16)10-12(15(18)21-24(7,8)9)11-14(17)20-23(4,5)
<b>InchiKey:</b>	RHDPKJMZPKZKTA-UHFFFAOYSA-N
<b>Formula:</b>	C15H30O6Si3
<b>SMILES:</b>	<chem>C[Si](C)(C)OC(=O)C=C(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C</chem>
<b>Mol. weight [g/mol]:</b>	390.65
<b>CAS:</b>	55887-88-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.30		Crippen Method
logp	3.437		Crippen Method
rinpol	1765.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1749.60		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1749.60		NIST Webbook
rinpol	1765.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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=C55887882&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55887882&amp;Units=SI</a>

# Legend

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

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