

1-Propene-1,2,3-tricarboxylic acid, tris(trimethylsilyl) ester, (E)-

Other names:

trans-Aconitic acid (3TMS)
(E)-Aconitic acid, tris-TMS
(E)-Aconitic acid, TMS
trans-Aconitic acid, tris(trimethylsilyl) ester
trans-Aconitic acid, TMS
Aconitic acid, (e)-, 3tms derivative

Inchi:

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,

InchiKey:

RHDPKJMZPKZKTA-ZRDIBKRKSA-N

Formula:

C15H30O6Si3

SMILES:

C[Si](C)(C)OC(=O)C=C(CC(=O)O[Si](C)(C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

390.65

CAS:

55530-72-8

Physical Properties

Property code	Value	Unit	Source
log10ws	3.30		Crippen Method
logp	3.437		Crippen Method
rinpol	1754.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1729.80		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1729.80		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530728&Units=SI>

Legend

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

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