

2-Hexenedioic acid, 2-[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester

Other names: Bis(trimethylsilyl) 2-[(trimethylsilyl)oxy]-2-hexenedioate

2-Ketoadipic acid, enol, tri-TMS

2-Ketoadipic acid, TMS

Inchi: InChI=1S/C15H32O5Si3/c1-21(2,3)18-13(15(17)20-23(7,8)9)11-10-12-14(16)19-22(4,5)6

InchiKey: SXIRXGDGZGVWMJ-QBFSEMIESA-N

Formula: C₁₅H₃₂O₅Si₃

SMILES: C[Si](C)(C)OC(=O)CCC=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 376.67

CAS: 55334-16-2

Physical Properties

Property code	Value	Unit	Source
log10ws	2.58		Crippen Method
logp	4.258		Crippen Method
rinpol	1712.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1712.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334162&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

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