

3-Ketoadipic acid, enol, tri-TMS

Other names: 3-Hydroxyhex-2-enedioic acid, trimethylsilyl ether, bis(trimethylsilyl) ester
Inchi: InChI=1S/C15H32O5Si3/c1-21(2,3)18-13(12-15(17)20-23(7,8)9)10-11-14(16)19-22(4,5)6
InchiKey: MZWJNCLLARMEMP-SEYXRHQNSA-N
Formula: C₁₅H₃₂O₅Si₃
SMILES: C[Si](C)(C)OC(=O)C=C(CCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 376.67
CAS: 72378-92-8

Physical Properties

Property code	Value	Unit	Source
log10ws	2.58		Crippen Method
logp	4.258		Crippen Method
rinpol	1739.00		NIST Webbook
rinpol	1704.30		NIST Webbook
rinpol	1704.30		NIST Webbook
rinpol	1739.00		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=C72378928&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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<https://www.chemeo.com/cid/125-222-6/3-Ketoadipic-acid-enol-tri-TMS.pdf>

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