

3-Ketoadipic acid, TMS # 2

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: IMVBPBMPWMKINR-RAXLEYEMSA-N
Formula: C15H32O5Si3
SMILES: C[Si](C)(C)OC(=O)CC=C(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 376.67

Physical Properties

Property code	Value	Unit	Source
log10ws	2.58		Crippen Method
logp	4.258		Crippen Method
rinpol	1673.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400570&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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.chemeo.com/cid/115-782-6/3-Ketoadipic-acid-TMS-2.pdf>

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