

3-Ketoadipic acid, TMS # 1

Inchi: InChI=1S/C12H24O5Si2/c1-18(2,3)16-11(14)8-7-10(13)9-12(15)17-19(4,5)6/h7-9H2,1-6H1
InchiKey: DOEYEWCTCLMKDV-UHFFFAOYSA-N
Formula: C12H24O5Si2
SMILES: C[Si](C)(C)OC(=O)CCC(=O)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 304.49

Physical Properties

Property code	Value	Unit	Source
log10ws	2.05		Crippen Method
logp	2.482		Crippen Method
rinpol	1709.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400565&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.cheméo.com/cid/14-712-5/3-Ketoadipic-acid-TMS-1.pdf>

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