

2-Ketoglutaric acid, TMS # 1

Inchi: InChI=1S/C11H22O5Si2/c1-17(2,3)15-10(13)8-7-9(12)11(14)16-18(4,5)6/h7-8H2,1-6H3
InchiKey: SIKHZPCWBUXAKA-UHFFFAOYSA-N
Formula: C11H22O5Si2
SMILES: C[Si](C)(C)OC(=O)CCC(=O)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 290.46
CAS: 1027138-06-2

Physical Properties

Property code	Value	Unit	Source
log10ws	2.47		Crippen Method
logp	2.092		Crippen Method
rinpol	1620.00		NIST Webbook
rinpol	1621.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1027138062&Units=SI>

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/19-771-5/2-Ketoglutaric-acid-TMS-1.pdf>

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