

Oxaloacetic acid, MO TBDMS # 2

Inchi: InChI=1S/C22H46O5Si3/c1-20(2,3)28(10,11)25-17(19(24)27-30(14,15)22(7,8)9)16-18(23)
InchiKey: KPTKAWGLDFVNBA-UHFFFAOYSA-N
Formula: C22H46O5Si3
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C=C(O[Si](C)(C)C(C)(C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 474.85

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.35 | | Crippen Method |
| logp | 6.989 | | Crippen Method |
| rinpol | 1897.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R564753&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/40-261-7/Oxaloacetic-acid-MO-TBDMS-2.pdf>

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