

Mannaric acid, TMS

Inchi: InChI=1S/C24H58O8Si6/c1-33(2,3)27-19(21(29-35(7,8)9)23(25)31-37(13,14)15)20(28-30)16-18
InchiKey: AFNUGMFTFWKGLV-CMOCDZPBSA-N
Formula: C₂₄H₅₈O₈Si₆
SMILES: C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 643.23

Physical Properties

Property code	Value	Unit	Source
log10ws	7.30		Crippen Method
logp	6.623		Crippen Method
rinsol	2026.00		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=R101872&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinsol: Non-polar retention indices

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<https://www.cheméo.com/cid/21-177-2/Mannaric-acid-TMS.pdf>

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