

Altronic acid, hexakis-TMS

Inchi: InChI=1S/C24H60O7Si6/c1-32(2,3)26-19-20(27-33(4,5)6)21(28-34(7,8)9)22(29-35(10,11)36)31(37-43(12,13)44)30(45-51(14,15)52)23(53-59(16,17)60)24(61-67(18,19)68)25(69-75(20,21)76)77(78,79)80

InchiKey: IVIMVRAMMWQMhj-ODAXIHTASA-N

Formula: C₂₄H₆₀O₇Si₆

SMILES: C[Si](C)(C)OCC(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[S

Mol. weight [g/mol]: 629.24

Physical Properties

Property code	Value	Unit	Source
log10ws	7.08		Crippen Method
logp	7.096		Crippen Method
rinpol	2061.00		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=R101570&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.cheméo.com/cid/15-872-7/Altronic-acid-hexakis-TMS.pdf>

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