

D-Quebrachitol, TMS

Inchi:	InChI=1S/C22H54O6Si5/c1-23-17-18(24-29(2,3)4)20(26-31(8,9)10)22(28-33(14,15)16)2
InchiKey:	IKOVCQNLJNHSBD-YGBDOONVSA-N
Formula:	C22H54O6Si5
SMILES:	COC1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]:	555.09

Physical Properties

Property code	Value	Unit	Source
log10ws	5.62		Crippen Method
logp	6.115		Crippen Method
rinpol	1911.00		NIST Webbook
rinpol	1918.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R532008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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/42-101-2/D-Quebrachitol-TMS.pdf>

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