

Adonitol (Ribitol), TMS

Other names:	Adonitol, pentakis(trimethylsilyl) ether
Inchi:	InChI=1S/C20H52O5Si5/c1-26(2,3)21-16-18(23-28(7,8)9)20(25-30(13,14)15)19(24-29(10,11)12)31-32(33,34)35
InchiKey:	SUZLPERYXSOGNY-UHFFFAOYSA-N
Formula:	C ₂₀ H ₅₂ O ₅ Si ₅
SMILES:	C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	513.05

Physical Properties

Property code	Value	Unit	Source
log10ws	5.78		Crippen Method
logp	6.350		Crippen Method
rinpol	1756.00		NIST Webbook
rinpol	1698.90		NIST Webbook
rinpol	1698.90		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/70-057-1/Adonitol-Ribitol-TMS.pdf>

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