

Arabitol, pentakis(trimethylsilyl)-

Other names:	1,2,3,4,5-Pentakis-O-(trimethylsilyl)arabitol Arabinitol, pentakis-TMS Arabitol (5TMS) Arabinitol, TMS Arabitol, TMS Arabinitol, 5tms derivative
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)17
InchiKey:	SUZLPERYXSOGNY-RTBURBONSA-N
Formula:	C20H52O5Si5
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
CAS:	14199-73-6

Physical Properties

Property code	Value	Unit	Source
log10ws	5.78		Crippen Method
logp	6.350		Crippen Method
rinpol	1758.70		NIST Webbook
rinpol	1702.30		NIST Webbook
rinpol	1718.90		NIST Webbook
rinpol	1737.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1748.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14199736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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