

«beta»-Galactopyranose, TMS

Other names:	«beta»-Galactose, TMS
Inchi:	InChI=1S/C21H52O6Si5/c1-28(2,3)22-16-17-18(24-29(4,5)6)19(25-30(7,8)9)20(26-31(10
InchiKey:	PPFHNIVPOLWPCF-XIYVOTBMSA-N
Formula:	C ₂₁ H ₅₂ O ₆ Si ₅
SMILES:	C[Si](C)(C)OCC1OC(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]:	541.06
CAS:	32166-97-5

Physical Properties

Property code	Value	Unit	Source
log10ws	5.66		Crippen Method
logp	6.075		Crippen Method
rinpol	1941.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1952.00		NIST Webbook
ripol	1869.00		NIST Webbook
ripol	1869.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32166975&Units=SI

Legend

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

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<https://www.cheméo.com/cid/41-398-5/beta-Galactopyranose-TMS.pdf>

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