

C-(erythro-1,2,3-trihydroxypropyl)glyceraric acid, TMS

Inchi:	InChI=1S/C24H58O8Si6/c1-33(2,3)27-19-20(28-34(4,5)6)21(29-35(7,8)9)24(32-38(16,17
InchiKey:	PEUWEFJXHJKYKW-SFTDATJTSA-N
Formula:	C24H58O8Si6
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)O[Si](C)(C)C)C(=O
Mol. weight [g/mol]:	643.23

Physical Properties

Property code	Value	Unit	Source
log10ws	7.42		Crippen Method
logp	6.625		Crippen Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R101634&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

Latest version available from:

<https://www.cheméo.com/cid/23-317-4/C-erythro-1-2-3-trihydroxypropyl-glyceraric-acid-TMS.pdf>

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