

D-galacturonic acid, TMS diethyldithioacetal derivative

Inchi:	InChI=1S/C25H60O6S2Si5/c1-18-32-25(33-19-2)23(30-37(12,13)14)21(28-35(6,7)8)20(2
InchiKey:	FOIFFUJOBWXFIH-WZYRSQIMSA-N
Formula:	C25H60O6S2Si5
SMILES:	CCSC(SCC)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](
Mol. weight [g/mol]:	661.30

Physical Properties

Property code	Value	Unit	Source
log10ws	3.42		Crippen Method
logp	8.077		Crippen Method
rinpol	2296.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/25-218-2/D-galacturonic-acid-TMS-diethyldithioacetal-derivative.pdf>

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