

Propyl glucuronide, TMS

Inchi: InChI=1S/C21H48O7Si4/c1-14-15-23-21-19(27-31(8,9)10)17(26-30(5,6)7)16(25-29(2,3)4)
InchiKey: RGPXUCUWGYNNC-UHFFFAOYSA-N
Formula: C₂₁H₄₈O₇Si₄
SMILES: CCCOC1OC(C(=O)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]: 524.94

Physical Properties

Property code	Value	Unit	Source
log10ws	3.94		Crippen Method
logp	5.176		Crippen Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R554677&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

Latest version available from:

<https://www.chemeo.com/cid/119-090-0/Propyl-glucuronide-TMS.pdf>

Generated by Cheméo on 2024-05-01 03:48:35.805137265 +0000 UTC m=+16824564.725714578.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.