

(S)-2-Methylbutyl glucuronide, TMS

Inchi: InChI=1S/C23H52O7Si4/c1-15-17(2)16-25-23-21(29-33(9,10)11)19(28-32(6,7)8)18(27-3
InchiKey: SZYCQSAICIJTNG-BBEXFNLESA-N
Formula: C23H52O7Si4
SMILES: CCC(C)COC1OC(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]: 553.00

Physical Properties

Property code	Value	Unit	Source
log10ws	3.34		Crippen Method
logp	5.812		Crippen Method
rinpol	2187.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R554791&Units=SI>

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/25-955-4/S-2-Methylbutyl-glucuronide-TMS.pdf>

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