

Isobutyl glucuronide, TMS

Inchi: InChI=1S/C22H50O7Si4/c1-16(2)15-24-22-20(28-32(9,10)11)18(27-31(6,7)8)17(26-30(3,4)25)21-23
InchiKey: VSRFFEPYOAWEU-UHFFFAOYSA-N
Formula: C₂₂H₅₀O₇Si₄
SMILES: CC(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]: 538.97

Physical Properties

Property code	Value	Unit	Source
log10ws	3.76		Crippen Method
logp	5.422		Crippen Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		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=R554513&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/114-240-8/Isobutyl-glucuronide-TMS.pdf>

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