

(R)-2-Butyl glucuronide, TMS

Inchi: InChI=1S/C22H50O7Si4/c1-15-16(2)24-22-20(28-32(9,10)11)18(27-31(6,7)8)17(26-30(3)
InchiKey: BYQDUSVVYSRQEK-DXYSLGBVSA-N
Formula: C22H50O7Si4
SMILES: CCC(C)OC1OC(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
logp	5.565		Crippen Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R554711&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/124-814-0/R-2-Butyl-glucuronide-TMS.pdf>

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