

Ethyl glucuronide, TMS

Inchi: InChI=1S/C20H46O7Si4/c1-14-22-20-18(26-30(8,9)10)16(25-29(5,6)7)15(24-28(2,3)4)17
InchiKey: ZVFLDYSKELVZGO-UHFFFAOYSA-N
Formula: C20H46O7Si4
SMILES: CCOC1OC(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]: 510.92

Physical Properties

Property code	Value	Unit	Source
log10ws	4.35		Crippen Method
logp	4.786		Crippen Method
rinsol	2019.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R554479&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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/22-690-1/Ethyl-glucuronide-TMS.pdf>

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