

Glucuronic acid, TMS # 3

Inchi: InChI=1S/C21H50O7Si5/c1-29(2,3)24-17(16-22)18(25-30(4,5)6)19(26-31(7,8)9)20(27-32)
InchiKey: HDGFBGPNRURMOV-IYWMVGAKSA-N
Formula: C21H50O7Si5
SMILES: C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C=O)O[Si](C)(C)C
Mol. weight [g/mol]: 555.04

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 6.19 | | Crippen Method |
| logp | 5.444 | | Crippen Method |
| rinpol | 2029.00 | | NIST Webbook |
| rinpol | 2029.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400936&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/32-163-5/Glucuronic-acid-TMS-3.pdf>

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