

Ethanol, trichloro, glucuronide, TMS

Inchi: InChI=1S/C20H45Cl3O6Si4/c1-30(2,3)25-13-15-16(27-31(4,5)6)17(28-32(7,8)9)18(29-33)
InchiKey: GRZKOIVLDGHGAT-POEJNWFMSA-N
Formula: C20H45Cl3O6Si4
SMILES: C[Si](C)(C)OCC1OC(OCC(Cl)(Cl)Cl)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 600.27

Physical Properties

Property code	Value	Unit	Source
log10ws	2.57		Crippen Method
logp	6.610		Crippen Method
rinpol	2296.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R112971&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/32-880-9/Ethanol-trichloro-glucuronide-TMS.pdf>

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