

Phloroglucinic acid, 4TMS

Inchi: InChI=1S/C19H38O5Si4/c1-25(2,3)21-15-13-16(22-26(4,5)6)18(19(20)24-28(10,11)12)17
InchiKey: UEYBDMIEPBZEAR-UHFFFAOYSA-N
Formula: C19H38O5Si4
SMILES: C[Si](C)(C)OC(=O)c1c(O[Si](C)(C)C)cc(O[Si](C)(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 458.84
CAS: 955381-58-5

Physical Properties

Property code	Value	Unit	Source
log10ws	2.37		Crippen Method
logp	6.319		Crippen Method
rinsol	1964.30		NIST Webbook
rinsol	1964.30		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C955381585&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/119-038-8/Phloroglucinic-acid-4TMS.pdf>

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