

cis-Coutaric acid, 4TMS

Inchi: InChI=1S/C25H44O8Si4/c1-34(2,3)30-20-16-13-19(14-17-20)15-18-21(26)29-22(24(27)30)23-25
InchiKey: UXTFDOZVFZVLZAV-SDXDJHTJSA-N
Formula: C25H44O8Si4
SMILES: C[Si](C)(C)OC(=O)C(OC(=O)C=Cc1ccc(O[Si](C)(C)C)cc1)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 584.95

Physical Properties

Property code	Value	Unit	Source
log10ws	2.79		Crippen Method
logp	5.802		Crippen Method
rinpol	2578.80		NIST Webbook
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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=U414026&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/83-941-5/cis-Coutaric-acid-4TMS.pdf>

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