

benzyl glucosinolate, TMS

Inchi: InChI=1S/C29H59NO9S2Si5/c1-42(2,3)33-22-24-26(35-43(4,5)6)27(36-44(7,8)9)28(37-4
InchiKey: OZIWGMJWBKNOBG-UHFFFAOYSA-N
Formula: C29H59NO9S2Si5
SMILES: C[Si](C)(C)OCC1OC(SC(Cc2ccccc2)=NOS(=O)(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)
Mol. weight [g/mol]: 770.34

Physical Properties

Property code	Value	Unit	Source
log10ws	2.77		Crippen Method
logp	7.625		Crippen Method
rinqol	2700.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R384002&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
rinqol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/55-439-4/benzyl-glucosinolate-TMS.pdf>

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