

Homogentisic acid, TBDMS

Other names: Homogentisic acid, bis(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester
Homogentisic acid, triTBDMS

Inchi: InChI=1S/C26H50O4Si3/c1-24(2,3)31(10,11)28-21-16-17-22(29-32(12,13)25(4,5)6)20(18)

InchiKey: VRJWMCKJWGZEFL-UHFFFAOYSA-N

Formula: C26H50O4Si3

SMILES: CC(C)(C)[Si](C)(C)OC(=O)Cc1cc(O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 510.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	8.546		Crippen Method
rinpol	2507.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2508.00		NIST Webbook
rinpol	2512.00		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2507.00		NIST Webbook
rinpol	2508.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U221799&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/28-595-1/Homogentisic-acid-TBDMS.pdf>

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