

1,3-Benzenediol, 4,6-dichloro, bis-TMS

Inchi: InChI=1S/C12H20Cl2O2Si2/c1-17(2,3)15-11-8-12(16-18(4,5)6)10(14)7-9(11)13/h7-8H,1-6H3
InchiKey: LPWIXFBBPJVSKU-UHFFFAOYSA-N
Formula: C12H20Cl2O2Si2
SMILES: C[Si](C)(C)Oc1cc(O[Si](C)(C)C)c(Cl)cc1Cl
Mol. weight [g/mol]: 323.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	5.421		Crippen Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R99816&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/118-505-0/1-3-Benzenediol-4-6-dichloro-bis-TMS.pdf>

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