

1,2-Cyclohexanediol, TMS

Inchi: InChI=1S/C12H28O2Si2/c1-15(2,3)13-11-9-7-8-10-12(11)14-16(4,5)6/h11-12H,7-10H2,1
InchiKey: XQTPMHWHLDRJLV-UHFFFAOYSA-N
Formula: C₁₂H₂₈O₂Si₂
SMILES: C[Si](C)(C)OC1CCCCC1O[Si](C)(C)C
Mol. weight [g/mol]: 260.52

Physical Properties

Property code	Value	Unit	Source
log10ws	0.76		Crippen Method
logp	4.001		Crippen Method
rinpol	1262.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R504944&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/24-397-5/1-2-Cyclohexanediol-TMS.pdf>

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