

2,5-Anhydrotalonic acid, TMS

Inchi: InChI=1S/C18H42O6Si4/c1-25(2,3)20-13-14-15(22-26(4,5)6)16(23-27(7,8)9)17(21-14)18
InchiKey: MIYOGWZXYKUMKR-YYIAUSFCSA-N
Formula: C18H42O6Si4
SMILES: C[Si](C)(C)OCC1OC(C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 466.86

Physical Properties

Property code	Value	Unit	Source
log10ws	4.89		Crippen Method
logp	4.424		Crippen Method
rinpol	1890.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R100775&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/52-539-6/2-5-Anhydrotalonic-acid-TMS.pdf>

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