

D-xylose, TMS diethyldithioacetal derivative

Inchi: InChI=1S/C21H52O4S2Si4/c1-15-26-21(27-16-2)20(25-31(12,13)14)19(24-30(9,10)11)1
InchiKey: SXKRVWDTTZYHFP-HSALFYBXSA-N
Formula: C21H52O4S2Si4
SMILES: CCSC(SCC)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 545.11

Physical Properties

Property code	Value	Unit	Source
log10ws	2.12		Crippen Method
logp	7.330		Crippen Method
rinpol	2120.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R502824&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/53-659-2/D-xylose-TMS-diethyldithioacetal-derivative.pdf>

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