

12-Docosenol, TMS

Inchi: InChI=1S/C25H52OSi/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey: DQEMWSKAMMGJQU-BUHFOSPRSA-N
Formula: C25H52OSi
SMILES: CCCCCCCCCC=CCCCCCCCCCCCCO[Si](C)(C)C
Mol. weight [g/mol]: 396.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.28		Crippen Method
logp	9.436		Crippen Method
rinpol	2524.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R166651&Units=SI>

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/86-660-4/12-Docosenol-TMS.pdf>

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