

Falcarinol, TMS

Inchi: InChI=1S/C20H32OSi/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-20(7-2)21-22(3,4)5/h7,11-13,15-17,19,21-22
InchiKey: WDWDEHVCHBVQLN-YPKPFQOOSA-N
Formula: C20H32OSi
SMILES: C=CC(C#CC#CCC=CCCCCCC)O[Si](C)(C)C
Mol. weight [g/mol]: 316.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	5.706		Crippen Method
rinpol	2080.70		NIST Webbook

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=U414697&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/77-577-7/Falcarinol-TMS.pdf>

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