

2-Nonenal, 3-hydroxy, TMS, PFBO, # 1

Inchi: InChI=1S/C19H26F5NO2Si/c1-5-6-7-8-9-13(27-28(2,3)4)10-11-25-26-12-14-15(20)17(22)
InchiKey: SEAQAZBLPDXFHC-FHVOTVFWSA-N
Formula: C19H26F5NO2Si
SMILES: CCCCCC(=CC=NOCc1c(F)c(F)c(F)c(F)c1F)O[Si](C)(C)C
Mol. weight [g/mol]: 423.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.76		Crippen Method
logp	6.590		Crippen Method
rinpol	1966.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R398873&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/33-279-6/2-Nonenal-3-hydroxy-TMS-PFBO-1.pdf>

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