Succinylacetone, O-pentafluorobenzyloxime, TMS

Inchi: InChI=1S/C24H22F10N2O4Si/c1-10(35-38-8-12-15(25)19(29)23(33)20(30)16(12)26)7-11

InchiKey: SYVIKTYZHWOGPK-OZQSKDJKSA-N

Formula: C24H22F10N2O4Si

SMILES: CC(CC(CCC(=O)O[Si](C)(C)C)=NOCc1c(F)c(F)c(F)c(F)c1F)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 620.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.78		Crippen Method
logp	7.091		Crippen Method
rinpol	2434.00		NIST Webbook
rinpol	2446.00		NIST Webbook
rinpol	2461.00		NIST Webbook
rinpol	2497.00		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=R315378&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/33-071-6/Succinylacetone-O-pentafluorobenzyloxime-TMS.pdf

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