

2-Ketoglutaric acid pfbo-tms

Other names:	2-Ketopentanedioic acid pfbo-tms 2-Oxoglutaric acid, O-pentafluorobenzyloxime, TMS
Inchi:	InChI=1S/C18H24F5NO5Si2/c1-30(2,3)28-12(25)8-7-11(18(26)29-31(4,5)6)24-27-9-10-1
InchiKey:	NBAOCXSOVAPOGN-UHFFFAOYSA-N
Formula:	C18H24F5NO5Si2
SMILES:	C[Si](C)(C)OC(=O)CCC(=NOCc1c(F)c(F)c(F)c1F)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	485.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	4.791		Crippen Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332303&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/117-404-3/2-Ketoglutaric-acid-pfbo-tms.pdf>

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