SEBACIC ACID diTBDMS

Other names:	Sebacic acid, bis(tert-butyldimethylsilyl) ester
	Sebacic acid, diTBDMS
	Sebacic acid, DMTBS
	Sebacic acid, TBDMS
	Bis[tert-butyl(dimethyl)silyl] sebacate
	Sebacic acid, 2tbdms derivative
Inchi:	InChI=1S/C22H46O4Si2/c1-21(2,3)27(7,8)25-19(23)17-15-13-11-12-14-16-18-20(24)26-2
InchiKey:	XANNRUSHAVBUKW-UHFFFAOYSA-N
Formula:	C22H46O4Si2
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)CCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	430.78

Physical Properties

Property code	Value	Unit	Source
hvap	85.18	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.44		Cheméo Relay (1.0)
logp	7.204		Crippen Method
pc	995.31	kPa	Cheméo Relay (1.0, beta)
rinpol	2378.00		NIST Webbook
rinpol	2366.70		NIST Webbook
rinpol	2372.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2372.00		NIST Webbook
rinpol	2366.70		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	590.05	K	Cheméo Relay (1.0)
tc	807.54	K	Cheméo Relay (1.0)
tf	344.39	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255983&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point