

BETA-LACTATE DI-TMS

Other names:	3-Trimethylsilyloxypropionic acid, trimethylsilyl ester «beta»-Lactate di-TMS 3-Hydroxypropionic acid, diTMS Propanoic acid, 3-hydroxy, di-TMS «beta»-Lactic acid, bis-TMS 3-Hydroxypropanoic acid, TMS 3-Hydroxypropionic acid, TMS Hydracrylic acid, 2tms derivative
Inchi:	InChI=1S/C9H22O3Si2/c1-13(2,3)11-8-7-9(10)12-14(4,5)6/h7-8H2,1-6H3
InchiKey:	IHW RJZSKTAMEMR-UHFFFAOYSA-N
Formula:	C9H22O3Si2
SMILES:	C[Si](C)(C)OCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	234.44

Physical Properties

Property code	Value	Unit	Source
hvap	57.04	kJ/mol	Cheméo Relay (1.0)
logp	2.606		Crippen Method
rinpol	1140.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1144.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55162328&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

h_{vap}: Enthalpy of vaporization at standard conditions
log_p: Octanol/Water partition coefficient
rin_{pol}: Non-polar retention indices

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