3-Hydroxyadipic acid, lactone, mono-TMS

Other names: 3-Hydroxyadipic acid, lactone, mono-TMS
Inchi: InChI=1S/C9H16O4Si/c1-14(2,3)13-9(11)6-7-4-5-8(10)12-7/h7H,4-6H2,1-3H3
InchiKey: RASUFFJSOATALI-UHFFFAOYSA-N
Formula: C9H16O4Si
SMILES: C[Si](C)(C)OC(=O)CC1CCC(=O)O1
Mol. weight [g/mol]: 216.31

Physical Properties

Property code	Value	Unit	Source
hf	-912.36	kJ/mol	Cheméo Relay (1.0)
hvap	69.80	kJ/mol	Cheméo Relay (1.0)
logp	1.460		Crippen Method
rinpol	1493.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1493.00		NIST Webbook
tb	547.12	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R164239&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):

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature