

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

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