

1,3,5-Trisilacyclohexane, 1,1,3,3,5,5-hexamethyl-

Other names: 1,1,3,3,5,5-Hexamethylcyclotrimethylenetrisilane

1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane

InChI: InChI=1S/C9H24Si3/c1-10(2)7-11(3,4)9-12(5,6)8-10/h7-9H2,1-6H3

InChIKey: ICSWLKDKQBNKAY-UHFFFAOYSA-N

Formula: C9H24Si3

SMILES: C[Si]1(C)C[Si](C)(C)C[Si](C)(C)C1

Mol. weight [g/mol]: 216.54

CAS: 1627-99-2

Physical Properties

Property code	Value	Unit	Source
ie	9.39 ± 0.03	eV	NIST Webbook
log10ws	3.85		Crippen Method
logp	3.743		Crippen Method
ss	477.39	J/mol×K	NIST Webbook
tt	269.28 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	400.95	J/mol×K	298.15	NIST Webbook
hfust	16.50	kJ/mol	269.28	NIST Webbook
hfust	16.50	kJ/mol	269.30	NIST Webbook
hvapt	45.52	kJ/mol	476.55	NIST Webbook
sfust	61.42	J/mol×K	269.28	NIST Webbook
svapt	95.52	J/mol×K	476.55	NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1627992&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
svapt:	Entropy of vaporization at a given temperature
tt:	Triple Point Temperature

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