1,1-Dimethyl-1-silacyclobutane

Other names: Silacyclobutane, 1,1-dimethyl-
Cyclotrimethylenedimethylsilane
1,1-Dimethylsilacyclobutane
Inchi: InChI=1S/C5H12Si/c1-6(2)4-3-5-6/h3-5H2,1-2H3
InchiKey: YQQFFTNDQFUNHB-UHFFFAOYSA-N
Formula: C5H12Si
SMILES: C[Si]1(C)CCC1
Mol. weight [g/mol]: 100.23
CAS: 2295-12-7

Physical Properties

Property code	Value	Unit	Source
hvap	33.00 ± 0.80	kJ/mol	NIST Webbook
ie	8.83 ± 0.07	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.97 ± 0.03	eV	NIST Webbook
ie	8.83 ± 0.07	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
log10ws	0.72		Crippen Method
logp	2.098		Crippen Method
ss	279.49	J/mol×K	NIST Webbook
tt	155.52 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	197.53	J/mol×K	298.15	NIST Webbook
hfust	6.76	kJ/mol	155.50	NIST Webbook
hfust	6.76	kJ/mol	155.52	NIST Webbook
hfust	6.76	kJ/mol	155.50	NIST Webbook
hvapt	32.14	kJ/mol	355.91	NIST Webbook
hvapt	32.10	kJ/mol	356.00	NIST Webbook
sfust	43.51	J/mol×K	155.52	NIST Webbook

sfust	42.87	J/mol×K	155.50	NIST Webbook
svapt	90.29	J/mol×K	355.91	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2295127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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