

Cyclotrisiloxane, hexamethyl-

Other names:	CH7260
	D3 (hexamethylcyclotrisiloxane)
	Dimethylsiloxane cyclic trimer
	Hexamethylcyclotrisiloxane
Inchi:	InChI=1S/C6H18O3Si3/c1-10(2)7-11(3,4)9-12(5,6)8-10/h1-6H3
InchiKey:	HTDJPCNNEPUOOQ-UHFFFAOYSA-N
Formula:	C6H18O3Si3
SMILES:	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O1
Mol. weight [g/mol]:	222.46
CAS:	541-05-9

Physical Properties

Property code	Value	Unit	Source
log10ws	4.61		Crippen Method
logp	2.155		Crippen Method
rinpol	827.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	831.00		NIST Webbook
ss	412.10	J/mol×K	NIST Webbook
tb	407.00	K	NIST Webbook
tf	339.50 ± 0.10	K	NIST Webbook
tf	337.00 ± 0.10	K	NIST Webbook
tt	335.22 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpl	420.10	J/mol×K	374.79	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	431.00	J/mol×K	400.00	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	430.00	J/mol×K	398.01	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	428.10	J/mol×K	393.14	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	425.60	J/mol×K	388.06	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	423.60	J/mol×K	383.15	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	421.80	J/mol×K	379.42	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	404.50	J/mol×K	339.90	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	405.90	J/mol×K	343.15	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane

cpl	406.70	J/mol×K	345.03	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	410.40	J/mol×K	353.15	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	412.30	J/mol×K	357.92	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	413.80	J/mol×K	361.20	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	415.60	J/mol×K	365.09	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	418.10	J/mol×K	370.16	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cpl	433.20	J/mol×K	404.89	Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane
cps	360.00	J/mol×K	298.15	NIST Webbook
hfust	16.61	kJ/mol	335.20	NIST Webbook
hsubt	55.20 ± 0.40	kJ/mol	316.00	NIST Webbook
hvapt	39.00	kJ/mol	373.00	NIST Webbook
hvapt	39.70	kJ/mol	378.00	NIST Webbook
hvapt	40.80	kJ/mol	380.50	NIST Webbook
hvapt	39.70	kJ/mol	365.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38637e+01
Coeff. B	-3.10902e+03
Coeff. C	-7.19820e+01
Temperature range (K), min.	300.99
Temperature range (K), max.	435.51

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane:	https://www.doi.org/10.1021/je050173+
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541059&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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