

Cyclotrisiloxane, hexaethyl-

Other names:	Hexaethylcyclotrisiloxane 1,1,3,3,5,5-Hexaethylcyclotrisiloxane
Inchi:	InChI=1S/C12H30O3Si3/c1-7-16(8-2)13-17(9-3,10-4)15-18(11-5,12-6)14-16/h7-12H2,1-6
InchiKey:	KMPBCFZCRNKXSA-UHFFFAOYSA-N
Formula:	C12H30O3Si3
SMILES:	CC[Si]1(CC)O[Si](CC)(CC)O[Si](CC)(CC)O1
Mol. weight [g/mol]:	306.62
CAS:	2031-79-0

Physical Properties

Property code	Value	Unit	Source
log10ws	2.10		Crippen Method
logp	4.496		Crippen Method
sl	674.71	J/molxK	NIST Webbook
sl	680.80	J/molxK	NIST Webbook
sl	674.40	J/molxK	NIST Webbook
tt	283.41 ± 0.02	K	NIST Webbook
tt	283.41 ± 0.02	K	NIST Webbook
tt	280.20 ± 0.10	K	NIST Webbook
tt	283.24 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	536.53	J/molxK	300.00	NIST Webbook
cpl	581.40	J/molxK	298.15	NIST Webbook
cpl	535.30	J/molxK	298.15	NIST Webbook
hfust	11.42	kJ/mol	280.20	NIST Webbook
hvapt	57.90	kJ/mol	454.50	NIST Webbook
hvapt	58.70	kJ/mol	475.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2031790&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpl: Liquid phase heat capacity
hfust: Enthalpy of fusion 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
sl: Liquid phase molar entropy at standard conditions
tt: Triple Point Temperature

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