Cyclopropane, 1,1,2,2-tetramethyl-

Other names: 1,1,2,2-Tetramethylcyclopropane
Inchi: InChI=1S/C7H14/c1-6(2)5-7(6,3)4/h5H2,1-4H3
InchiKey: JCHUCGKEGUAHEH-UHFFFAOYSA-N
Formula: C7H14
SMILES: CC1(C)CC1(C)C
Mol. weight [g/mol]: 98.19
CAS: 4127-47-3

Physical Properties

Property code	Value	Unit	Source
chl	-4635.62 ± 0.84	kJ/mol	NIST Webbook
gf	50.12	kJ/mol	Joback Method
hf	-104.87	kJ/mol	Joback Method
hfl	-119.80 ± 0.92	kJ/mol	NIST Webbook
hfus	0.50	kJ/mol	Joback Method
hvap	28.48	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.442		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	621.20		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	618.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	618.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	618.00		NIST Webbook
tb	349.00 ± 0.20	K	NIST Webbook

tb	349.00 ± 0.30	K	NIST Webbook
tb	349.00 ± 0.30	K	NIST Webbook
tb	349.04 ± 0.30	K	NIST Webbook
tb	349.00 ± 0.20	K	NIST Webbook
tc	556.59	K	Joback Method
tf	230.15	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.90	J/mol×K	362.11	Joback Method
cpg	193.91	J/mol×K	394.52	Joback Method
cpg	208.42	J/mol×K	426.94	Joback Method
cpg	221.59	J/mol×K	459.35	Joback Method
cpg	233.56	J/mol×K	491.76	Joback Method
cpg	244.49	J/mol×K	524.18	Joback Method
cpg	254.53	J/mol×K	556.59	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73089e+01
Coeff. B	-3.89273e+03
Coeff. C	-4.22570e+01
Temperature range (K), min.	270.96
Temperature range (K), max.	366.72

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4127473&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume