

Cyclopentane, 1,1,3,3-tetramethyl-

Other names:	1,1,3,3-Tetramethylcyclopentane
Inchi:	InChI=1S/C9H18/c1-8(2)5-6-9(3,4)7-8/h5-7H2,1-4H3
InchiKey:	YWYCGTZNHWYQBD-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CC1(C)CCC(C)(C)C1
Mol. weight [g/mol]:	126.24
CAS:	50876-33-0

Physical Properties

Property code	Value	Unit	Source
gf	42.76	kJ/mol	Joback Method
hf	-158.47	kJ/mol	Joback Method
hfus	1.48	kJ/mol	Joback Method
hvap	33.27	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	765.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	776.90		NIST Webbook
rinpol	772.80		NIST Webbook
rinpol	770.00		NIST Webbook
tb	391.11 ± 0.30	K	NIST Webbook
tb	391.19 ± 0.20	K	NIST Webbook
tc	624.78	K	Joback Method
tf	184.86 ± 0.30	K	NIST Webbook
tf	184.86 ± 0.30	K	NIST Webbook
tf	184.74 ± 0.30	K	NIST Webbook
tf	184.90 ± 1.00	K	NIST Webbook
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.55	J/molxK	416.41	Joback Method
cpg	276.80	J/molxK	451.14	Joback Method
cpg	294.48	J/molxK	485.87	Joback Method
cpg	310.77	J/molxK	520.59	Joback Method
cpg	325.84	J/molxK	555.32	Joback Method
cpg	339.87	J/molxK	590.05	Joback Method
cpg	353.03	J/molxK	624.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.18072e+01
Coeff. B	-2.68899e+03
Coeff. C	-4.85240e+01
Temperature range (K), min.	281.95
Temperature range (K), max.	462.49

Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

Crippen Method:

Joback Method:

KDB:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

<https://www.thermo.com/files/research/kdb/mol/mol548.mol>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C50876330&Units=SI>

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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

Latest version available from:

<https://www.cheméo.com/cid/16-179-6/Cyclopentane-1-1-3-3-tetramethyl.pdf>

Generated by Cheméo on 2024-04-18 05:47:17.37820229 +0000 UTC m=+15708486.298779602.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.