

Cyclohexene, 1,5,5-trimethyl-

Other names:	1,5,5-trimethylcyclohexene
Inchi:	InChI=1S/C9H16/c1-8-5-4-6-9(2,3)7-8/h5H,4,6-7H2,1-3H3
InchiKey:	CHOOCIQDWNAXQQ-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CC1=CCCC(C)(C)C1
Mol. weight [g/mol]:	124.22
CAS:	503-46-8

Physical Properties

Property code	Value	Unit	Source
chl	-5595.70	kJ/mol	NIST Webbook
gf	64.19	kJ/mol	Joback Method
hf	-113.22	kJ/mol	Joback Method
hfus	5.44	kJ/mol	Joback Method
hvap	35.86	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.143		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	884.00		NIST Webbook
tb	429.25	K	Joback Method
tc	640.93	K	Joback Method
tf	235.75	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.07	J/mol×K	429.25	Joback Method
cpg	261.48	J/mol×K	464.53	Joback Method
cpg	277.72	J/mol×K	499.81	Joback Method
cpg	292.91	J/mol×K	535.09	Joback Method
cpg	307.14	J/mol×K	570.37	Joback Method
cpg	320.51	J/mol×K	605.65	Joback Method

cpg

333.12

J/mol×K

640.93

Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35217e+01
Coeff. B	-3.27828e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	303.72
Temperature range (K), max.	455.30

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C503468&Units=SI>

The Yaws Handbook of Vapor

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

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>

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
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
mccol:	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

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