Propane, 1-chloro-2,2-dimethyl-

Other names:	1-Chloro-2,2-dimethylpropane
	Neopentyl chloride
	t-C4H9CH2Cl
Inchi:	InChI=1S/C5H11Cl/c1-5(2,3)4-6/h4H2,1-3H3
InchiKey:	JEKYMVBQWWZVHO-UHFFFAOYSA-N
Formula:	C5H11Cl
SMILES:	CC(C)(C)CCl
Mol. weight [g/mol]:	106.59
CAS:	753-89-9

Physical Properties

Property code	Value	Unit	Source
gf	-17.87	kJ/mol	Joback Method
hf	-171.02	kJ/mol	Joback Method
hfus	5.49	kJ/mol	Joback Method
hvap	29.81	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	2.271		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	644.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	654.00		NIST Webbook
tb	357.55 ± 0.70	K	NIST Webbook
tb	357.15 ± 1.50	K	NIST Webbook
tb	357.50	K	NIST Webbook
tc	532.51	K	Joback Method
tf	253.00 ± 4.00	K	NIST Webbook
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	151.66	J/mol×K	348.00	Joback Method
cpg	162.20	J/mol×K	378.75	Joback Method
cpg	172.18	J/mol×K	409.50	Joback Method
cpg	181.62	J/mol×K	440.25	Joback Method
cpg	190.56	J/mol×K	471.01	Joback Method
cpg	199.01	J/mol×K	501.76	Joback Method
cpg	207.00	J/mol×K	532.51	Joback Method
dvisc	0.0090043	Pa×s	178.45	Joback Method
dvisc	0.0036100	Pa×s	206.71	Joback Method
dvisc	0.0018032	Pa×s	234.97	Joback Method
dvisc	0.0010454	Pa×s	263.23	Joback Method
dvisc	0.0006737	Pa×s	291.48	Joback Method
dvisc	0.0004692	Pa×s	319.74	Joback Method
dvisc	0.0003465	Pa×s	348.00	Joback Method
hvapt	34.90	kJ/mol	337.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54494e+01
Coeff. B	-3.43323e+03
Coeff. C	-4.05210e+01
Temperature range (K), min.	253.15
Temperature range (K), max.	379.17

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C753899&Units=SI

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
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