Propane, 1,1,1,2-tetrachloro-2-methyl-

Other names: 1,1,1,2-tetrachloro-2-methylpropane
Inchi: InChI=1S/C4H6Cl4/c1-3(2,5)4(6,7)8/h1-2H3
InchiKey: PKPINLDBKJAFHQ-UHFFFAOYSA-N
Formula: C4H6Cl4
SMILES: CC(C)(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 195.90
CAS: 7086-07-9

Physical Properties

Property code	Value	Unit	Source
gf	-59.24	kJ/mol	Joback Method
hf	-206.35	kJ/mol	Joback Method
hfus	8.08	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.374		Crippen Method
mcvol	116.180	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	978.00		NIST Webbook
tb	434.18	K	Joback Method
tc	660.16	K	Joback Method
tf	452.30 ± 1.50	K	NIST Webbook
tf	452.25 ± 1.50	K	NIST Webbook
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.58	J/mol×K	434.18	Joback Method
cpg	199.43	J/mol×K	471.84	Joback Method
cpg	207.40	J/mol×K	509.51	Joback Method
cpg	214.54	J/mol×K	547.17	Joback Method
cpg	220.93	J/mol×K	584.84	Joback Method
cpg	226.65	J/mol×K	622.50	Joback Method

cpg	231.75	J/mol×K	660.16	Joback Method
dvisc	0.0077647	Pa×s	259.36	Joback Method
dvisc	0.0037729	Pa×s	288.50	Joback Method
dvisc	0.0020929	Pa×s	317.63	Joback Method
dvisc	0.0012818	Pa×s	346.77	Joback Method
dvisc	0.0008470	Pa×s	375.91	Joback Method
dvisc	0.0005941	Pa×s	405.04	Joback Method
dvisc	0.0004370	Pa×s	434.18	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	5.53851e+00
Coeff. B	-3.65455e+02
Coeff. C	-6.70210e+01
Temperature range (K), min.	136.62
Temperature range (K), max.	1676.85

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=C7086079&Units=SI

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
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