Propane, 1,2,2,3-tetrachloro-

Other names: 1,2,2,3-Tetrachloropropane
Inchi: InChI=1S/C3H4Cl4/c4-1-3(6,7)2-5/h1-2H2
InchiKey: UDPHJTAYHSSOQB-UHFFFAOYSA-N
Formula: C3H4Cl4
SMILES: ClCC(Cl)(Cl)CCl
Mol. weight [g/mol]: 181.88
CAS: 13116-53-5

Physical Properties

Property code	Value	Unit	Source
chl	-1594.90	kJ/mol	NIST Webbook
gf	-70.50	kJ/mol	Joback Method
hf	-176.96	kJ/mol	Joback Method
hfl	-252.10	kJ/mol	NIST Webbook
hfus	12.90	kJ/mol	Joback Method
hvap	38.52	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.638		Crippen Method
mcvol	102.090	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	963.00		NIST Webbook
tb	437.15 ± 1.50	K	NIST Webbook
tb	438.20	K	NIST Webbook
tb	438.00 ± 4.00	K	NIST Webbook
tc	628.09	K	Joback Method
tf	245.67	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.33	J/mol×K	414.53	Joback Method
cpg	158.61	J/mol×K	450.12	Joback Method
cpg	164.34	J/mol×K	485.72	Joback Method

cpg	169.58	J/mol×K	521.31	Joback Method
cpg	174.34	J/mol×K	556.90	Joback Method
cpg	178.66	J/mol×K	592.49	Joback Method
cpg	182.59	J/mol×K	628.09	Joback Method
dvisc	0.0057209	Pa×s	245.67	Joback Method
dvisc	0.0030305	Pa×s	273.81	Joback Method
dvisc	0.0018071	Pa×s	301.96	Joback Method
dvisc	0.0011770	Pa×s	330.10	Joback Method
dvisc	0.0008200	Pa×s	358.24	Joback Method
dvisc	0.0006021	Pa×s	386.39	Joback Method
dvisc	0.0004611	Pa×s	414.53	Joback Method
hvapt	42.80	kJ/mol	380.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	324.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43704e+01
Coeff. B	-3.66214e+03
Coeff. C	-6.26780e+01
Temperature range (K), min.	322.72
Temperature range (K), max.	466.93

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13116535&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume