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

Other names: 1,1,1,3-Tetrachloropropane
Inchi: InChI=1S/C3H4Cl4/c4-2-1-3(5,6)7/h1-2H2
InchiKey: UTACNSITJSJFHA-UHFFFAOYSA-N
Formula: C3H4Cl4
SMILES: ClCCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 181.88
CAS: 1070-78-6

Physical Properties

Property code	Value	Unit	Source
chl	-1638.00 ± 1.10	kJ/mol	NIST Webbook
gf	-70.50	kJ/mol	Joback Method
hf	-176.96	kJ/mol	Joback Method
hfl	-208.70 ± 1.10	kJ/mol	NIST Webbook
hfus	12.90	kJ/mol	Joback Method
hvap	38.52	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.986		Crippen Method
mcvol	102.090	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	921.00		NIST Webbook
rinpol	921.00		NIST Webbook
sl	284.30	J/mol×K	NIST Webbook
tb	432.00 ± 2.00	K	NIST Webbook
tb	430.90 ± 2.00	K	NIST Webbook
tb	432.20	K	NIST Webbook
tc	628.09	K	Joback Method
tf	245.67	K	Joback Method
tt	237.74 ± 0.02	K	NIST Webbook
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	182.59	J/mol×K	628.09	Joback Method
cpg	174.34	J/mol×K	556.90	Joback Method
cpg	169.58	J/mol×K	521.31	Joback Method
cpg	164.34	J/mol×K	485.72	Joback Method
cpg	158.61	J/mol×K	450.12	Joback Method
cpg	152.33	J/mol×K	414.53	Joback Method
cpg	178.66	J/mol×K	592.49	Joback Method
cpl	196.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0004611	Pa×s	414.53	Joback Method
dvisc	0.0011770	Pa×s	330.10	Joback Method
dvisc	0.0018071	Pa×s	301.96	Joback Method
dvisc	0.0030305	Pa×s	273.81	Joback Method
dvisc	0.0057209	Pa×s	245.67	Joback Method
dvisc	0.0008200	Pa×s	358.24	Joback Method
dvisc	0.0006021	Pa×s	386.39	Joback Method
hfust	10.49	kJ/mol	237.70	NIST Webbook
hfust	10.49	kJ/mol	237.70	NIST Webbook
hfust	2.20	kJ/mol	219.90	NIST Webbook
hvapt	57.80	kJ/mol	338.50	NIST Webbook
sfust	10.03	J/mol×K	219.90	NIST Webbook
sfust	44.13	J/mol×K	237.70	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.00 ± 1.00	K	7.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44427e+01
Coeff. B	-3.64398e+03
Coeff. C	-6.12880e+01
Temperature range (K), min.	318.72
Temperature range (K), max.	460.36

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1070786&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
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume