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

Other names: 1,1,1,2-Tetrachloropropane
CH3CHClCCl3
Inchi: InChI=1S/C3H4Cl4/c1-2(4)3(5,6)7/h2H,1H3
InchiKey: FEKGWIHDBVDVSM-UHFFFAOYSA-N
Formula: C3H4Cl4
SMILES: CC(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 181.88
CAS: 812-03-3

Physical Properties

Property code	Value	Unit	Source
gf	-72.94	kJ/mol	Joback Method
hf	-182.24	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	38.13	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.984		Crippen Method
mcvol	102.090	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	918.00		NIST Webbook
tb	414.09	K	Joback Method
tc	633.01	K	Joback Method
tf	209.00 ± 4.00	K	NIST Webbook
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.43	J/mol×K	414.09	Joback Method
cpg	158.97	J/mol×K	450.58	Joback Method
cpg	164.94	J/mol×K	487.06	Joback Method
cpg	170.36	J/mol×K	523.55	Joback Method
cpg	175.28	J/mol×K	560.04	Joback Method

cpg	179.73	J/mol×K	596.53	Joback Method
cpg	183.76	J/mol×K	633.01	Joback Method
dvisc	0.0088117	Pa×s	230.67	Joback Method
dvisc	0.0040006	Pa×s	261.24	Joback Method
dvisc	0.0021431	Pa×s	291.81	Joback Method
dvisc	0.0012923	Pa×s	322.38	Joback Method
dvisc	0.0008506	Pa×s	352.95	Joback Method
dvisc	0.0005985	Pa×s	383.52	Joback Method
dvisc	0.0004436	Pa×s	414.09	Joback Method
hvapt	42.30	kJ/mol	400.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.26725e+01
Coeff. B	-3.05911e+03
Coeff. C	-6.28950e+01
Temperature range (K), min.	309.90
Temperature range (K), max.	478.48

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C812033&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

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