

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

Other names:	1,1,2,3-Tetrachloropropane
Inchi:	InChI=1S/C3H4Cl4/c4-1-2(5)3(6)7/h2-3H,1H2
InchiKey:	BUQMVYQMVLAYRU-UHFFFAOYSA-N
Formula:	C3H4Cl4
SMILES:	CICC(Cl)C(Cl)Cl
Mol. weight [g/mol]:	181.88
CAS:	18495-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-78.22	kJ/mol	Joback Method
hf	-178.77	kJ/mol	Joback Method
hfus	13.27	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.636		Crippen Method
mcvol	102.090	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	453.15 ± 1.50	K	NIST Webbook
tc	626.28	K	Joback Method
tf	213.25	K	Joback Method
vc	0.388	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.81	J/mol×K	416.88	Joback Method
cpg	155.53	J/mol×K	451.78	Joback Method
cpg	160.89	J/mol×K	486.68	Joback Method
cpg	165.91	J/mol×K	521.58	Joback Method
cpg	170.61	J/mol×K	556.48	Joback Method
cpg	174.99	J/mol×K	591.38	Joback Method
cpg	179.08	J/mol×K	626.28	Joback Method
dvisc	0.0088171	Paxs	213.25	Joback Method

dvisc	0.0036878	Paxs	247.19	Joback Method
dvisc	0.0019038	Paxs	281.13	Joback Method
dvisc	0.0011333	Paxs	315.06	Joback Method
dvisc	0.0007462	Paxs	349.00	Joback Method
dvisc	0.0005291	Paxs	382.94	Joback Method
dvisc	0.0003968	Paxs	416.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43292e+01
Coeff. B	-3.75402e+03
Coeff. C	-6.65700e+01
Temperature range (K), min.	333.92
Temperature range (K), max.	482.86

Sources

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=C18495302&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/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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