

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

Other names:	1,1,2,2-Tetrachloropropane
Inchi:	InChI=1S/C3H4Cl4/c1-3(6,7)2(4)5/h2H,1H3
InchiKey:	MDCBRXYTSHYYJE-UHFFFAOYSA-N
Formula:	C3H4Cl4
SMILES:	CC(Cl)(Cl)C(Cl)Cl
Mol. weight [g/mol]:	181.88
CAS:	13116-60-4

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
tb	426.15 ± 1.50	K	NIST Webbook
tc	633.01	K	Joback Method
tf	230.67	K	Joback Method
vc	0.383	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.43	J/mol×K	414.09	Joback Method
cpg	179.73	J/mol×K	596.53	Joback Method
cpg	175.28	J/mol×K	560.04	Joback Method
cpg	170.36	J/mol×K	523.55	Joback Method
cpg	164.94	J/mol×K	487.06	Joback Method
cpg	158.97	J/mol×K	450.58	Joback Method
cpg	183.76	J/mol×K	633.01	Joback Method
dvisc	0.0004436	Paxs	414.09	Joback Method

dvisc	0.0005985	Paxs	383.52	Joback Method
dvisc	0.0008506	Paxs	352.95	Joback Method
dvisc	0.0012923	Paxs	322.38	Joback Method
dvisc	0.0021431	Paxs	291.81	Joback Method
dvisc	0.0040006	Paxs	261.24	Joback Method
dvisc	0.0088117	Paxs	230.67	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46141e+01
Coeff. B	-3.65818e+03
Coeff. C	-6.01760e+01
Temperature range (K), min.	315.52
Temperature range (K), max.	456.10

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C13116604&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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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