

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

Other names:	1,1,2,3-tetrachloro-2-methylpropane
Inchi:	InChI=1S/C4H6Cl4/c1-4(8,2-5)3(6)7/h3H,2H2,1H3
InchiKey:	WAURADWXPYHJJA-UHFFFAOYSA-N
Formula:	C4H6Cl4
SMILES:	CC(Cl)(CCl)C(Cl)Cl
Mol. weight [g/mol]:	195.90
CAS:	18963-01-4

Physical Properties

Property code	Value	Unit	Source
gf	-64.52	kJ/mol	Joback Method
hf	-202.88	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	40.35	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	3.026		Crippen Method
mcvol	116.180	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
rinpol	1047.00		NIST Webbook
tb	464.10 ± 2.00	K	NIST Webbook
tc	653.13	K	Joback Method
tf	227.00 ± 3.00	K	NIST Webbook
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.81	J/molxK	436.97	Joback Method
cpg	195.82	J/molxK	473.00	Joback Method
cpg	203.18	J/molxK	509.02	Joback Method
cpg	209.95	J/molxK	545.05	Joback Method
cpg	216.16	J/molxK	581.07	Joback Method
cpg	221.85	J/molxK	617.10	Joback Method
cpg	227.06	J/molxK	653.13	Joback Method

dvisc	0.0083832	Paxs	241.94	Joback Method
dvisc	0.0037365	Paxs	274.44	Joback Method
dvisc	0.0019762	Paxs	306.95	Joback Method
dvisc	0.0011808	Paxs	339.46	Joback Method
dvisc	0.0007720	Paxs	371.96	Joback Method
dvisc	0.0005404	Paxs	404.47	Joback Method
dvisc	0.0003989	Paxs	436.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44875e+01
Coeff. B	-3.88901e+03
Coeff. C	-7.00450e+01
Temperature range (K), min.	343.92
Temperature range (K), max.	493.87

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18963014&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
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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