

1-Propene, 1,2,3,3-tetrachloro-

Other names:	1,1,2,3-Tetrachloro-2-propene 1,2,3,3-Tetrachloro-1-propene 1,2,3,3-Tetrachloropropene Propene, 1,2,3,3-tetrachloro-
Inchi:	InChI=1S/C3H2Cl4/c4-1-2(5)3(6)7/h1,3H/b2-1-
InchiKey:	JUGQRTGGLWOBPG-UPHRSURJSA-N
Formula:	C3H2Cl4
SMILES:	ClC=C(Cl)C(Cl)Cl
Mol. weight [g/mol]:	179.86
CAS:	20589-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-4.11	kJ/mol	Joback Method
hf	-66.06	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	39.46	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.109		Crippen Method
mcvol	97.790	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	421.36	K	Joback Method
tc	641.14	K	Joback Method
tf	209.21	K	Joback Method
vc	0.374	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.27	J/mol×K	421.36	Joback Method
cpg	138.11	J/mol×K	457.99	Joback Method
cpg	142.53	J/mol×K	494.62	Joback Method
cpg	146.55	J/mol×K	531.25	Joback Method
cpg	150.20	J/mol×K	567.88	Joback Method

cpg	153.52	J/mol×K	604.51	Joback Method
cpg	156.54	J/mol×K	641.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.62835e+01
Coeff. B	-4.11091e+03
Coeff. C	-6.21220e+01
Temperature range (K), min.	319.12
Temperature range (K), max.	436.80

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=C20589859&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
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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