

Propane, 1,1,2,3,3-pentachloro-

Other names:	1,1,2,3,3-Pentachloropropane
Inchi:	InChI=1S/C3H3Cl5/c4-1(2(5)6)3(7)8/h1-3H
InchiKey:	PANVCEBTPSTUEL-UHFFFAOYSA-N
Formula:	C3H3Cl5
SMILES:	C1C(Cl)C(Cl)C(Cl)Cl
Mol. weight [g/mol]:	216.32
CAS:	15104-61-7

Physical Properties

Property code	Value	Unit	Source
gf	-92.59	kJ/mol	Joback Method
hf	-199.79	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.201		Crippen Method
mcvol	114.330	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinpol	1119.00		NIST Webbook
tb	472.20	K	NIST Webbook
tc	675.61	K	Joback Method
tf	228.17	K	Joback Method
vc	0.430	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.76	J/mol×K	453.87	Joback Method
cpg	192.37	J/mol×K	638.65	Joback Method
cpg	188.39	J/mol×K	601.69	Joback Method
cpg	184.06	J/mol×K	564.74	Joback Method
cpg	179.36	J/mol×K	527.78	Joback Method
cpg	174.27	J/mol×K	490.83	Joback Method
cpg	196.02	J/mol×K	675.61	Joback Method

dvisc	0.0003743	Paxs	453.87	Joback Method
dvisc	0.0005109	Paxs	416.25	Joback Method
dvisc	0.0007419	Paxs	378.64	Joback Method
dvisc	0.0011697	Paxs	341.02	Joback Method
dvisc	0.0020648	Paxs	303.40	Joback Method
dvisc	0.0042806	Paxs	265.79	Joback Method
dvisc	0.0112863	Paxs	228.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40858e+01
Coeff. B	-3.78501e+03
Coeff. C	-7.24080e+01
Temperature range (K), min.	346.72
Temperature range (K), max.	503.78

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15104617&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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