Pentane, 1,5-dichloro-

Other names:	1,5-Dichloropentane
	AMYLENE CHLORIDE
	PENTAMETHYLENE CHLORIDE
	Pentamethylene dichloride
Inchi:	InChI=1S/C5H10Cl2/c6-4-2-1-3-5-7/h1-5H2
InchiKey:	LBKDGROORAKTLC-UHFFFAOYSA-N
Formula:	C5H10Cl2
SMILES:	ClCCCCCCl
Mol. weight [g/mol]:	141.04
CAS:	628-76-2

Physical Properties

Property code	Value	Unit	Source
gf	-32.64	kJ/mol	Joback Method
hf	-178.01	kJ/mol	Joback Method
hfus	17.10	kJ/mol	Joback Method
hvap	52.20	kJ/mol	NIST Webbook
hvap	51.30 ± 0.80	kJ/mol	NIST Webbook
hvap	50.71	kJ/mol	NIST Webbook
log10ws	-2.22		Crippen Method
logp	2.634		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	3184.73	kPa	Joback Method
rinpol	1002.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1028.00		NIST Webbook
ripol	1444.00		NIST Webbook
tb	455.15 ± 0.50	K	NIST Webbook
tb	453.15 ± 1.00	K	NIST Webbook
tb	451.15 ± 2.00	K	NIST Webbook
tb	453.20	K	NIST Webbook
tc	569.78	K	Joback Method

tf	205.95	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.96	J/mol×K	449.03	Joback Method
cpg	175.74	J/mol×K	388.66	Joback Method
cpg	201.02	J/mol×K	479.22	Joback Method
cpg	208.73	J/mol×K	509.41	Joback Method
cpg	216.09	J/mol×K	539.60	Joback Method
cpg	223.13	J/mol×K	569.78	Joback Method
cpg	184.54	J/mol×K	418.85	Joback Method
cpl	211.89	J/mol×K	293.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	212.94	J/mol×K	298.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	209.65	J/mol×K	283.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	214.06	J/mol×K	303.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	215.21	J/mol×K	308.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}

cpl	216.38	J/mol×K	313.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	217.56	J/mol×K	318.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	218.76	J/mol×K	323.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	210.73	J/mol×K	288.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	213.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0003408	Pa×s	388.66	Joback Method
dvisc	0.0021944	Pa×s	236.40	Joback Method
dvisc	0.0012756	Pa×s	266.85	Joback Method
dvisc	0.0008286	Pa×s	297.30	Joback Method
dvisc	0.0005832	Pa×s	327.76	Joback Method
dvisc	0.0004357	Pa×s	358.21	Joback Method
dvisc	0.0044320	Pa×s	205.95	Joback Method
hvapt	47.20	kJ/mol	407.50	NIST Webbook
rfi	1.45400		298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I: HE and V E for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6
srf	0.04	N/m	293.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

srf	0.03	N/m	298.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	303.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	308.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	313.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.70	K	1.30	NIST Webbook
tbrp	336.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46842e+01
Coeff. B	-4.05298e+03
Coeff. C	-5.05550e+01
Temperature range (K), min.	332.08
Temperature range (K), max.	482.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.19870e+01

Coeff. B	-8.32410e+03
Coeff. C	-8.10746e+00
Coeff. D	2.89471e-06
Temperature range (K), min.	200.35
Temperature range (K), max.	663.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1617
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides)III. HE m and V E m for 20 binary mixtures {xCu-1H2u-1CO2C4H9 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 4, a = 1 and v = x ± 2 to 6:	https://www.doi.org/10.1016/j.jct.2005.11.003
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides)V: He and Vex for 25 binary mixtures {xCu-1H2u-1CO2CH3 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6:	https://www.doi.org/10.1016/j.jct.2006.10.008
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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat Capacities of alpha,omega-Dichloroalkanes at Temperatures from 284.15 K to 353.15 K and a Group Additivity Analysis:	https://www.doi.org/10.1021/je020042y
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII. HE m and VE m for 20 binary mixtures {xCu 1H2u 1CO2C3H7 + (1 x)a,x-ClCH2(CH2)v 2CH2Cl}, where u = 1 to 4, a = 1 and v = x = 2 to 6:	https://www.doi.org/10.1016/j.jct.2008.10.007
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628762&Units=SI
The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes: An analysis of behavior using the COSMO-RS methodology:	https://www.doi.org/10.1016/j.jct.2018.12.042
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I: HE and V E for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6:	https://www.doi.org/10.1016/j.jct.2005.03.020
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1617.mol
Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}:	https://www.doi.org/10.1021/je034177v

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating

nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume