Pentane, 1,4-dichloro-

Other names:	1,4-Dichloropentane
Inchi:	InChI=1S/C5H10Cl2/c1-5(7)3-2-4-6/h5H,2-4H2,1H3
InchiKey:	IJZUPZAYWWVHIO-UHFFFAOYSA-N
Formula:	C5H10Cl2
SMILES:	CC(Cl)CCCCl
Mol. weight [g/mol]:	141.04
CAS:	626-92-6

Physical Properties

Property code	Value	Unit	Source
gf	-35.08	kJ/mol	Joback Method
hf	-183.29	kJ/mol	Joback Method
hfus	13.58	kJ/mol	Joback Method
hvap	48.90	kJ/mol	NIST Webbook
hvap	48.10 ± 0.80	kJ/mol	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.633		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
ripol	1337.00		NIST Webbook
tb	435.15 ± 2.00	K	NIST Webbook
tc	573.69	K	Joback Method
tf	190.95	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.71	J/mol×K	388.22	Joback Method
cpg	184.82	J/mol×K	419.13	Joback Method
cpg	193.52	J/mol×K	450.04	Joback Method
cpg	201.84	J/mol×K	480.96	Joback Method

cpg	209.78	J/mol×K	511.87	Joback Method
cpg	217.36	J/mol×K	542.78	Joback Method
cpg	224.58	J/mol×K	573.69	Joback Method
dvisc	0.0072543	Pa×s	190.95	Joback Method
dvisc	0.0029682	Pa×s	223.83	Joback Method
dvisc	0.0015268	Pa×s	256.71	Joback Method
dvisc	0.0009134	Pa×s	289.59	Joback Method
dvisc	0.0006068	Pa×s	322.46	Joback Method
dvisc	0.0004348	Pa×s	355.34	Joback Method
dvisc	0.0003296	Pa×s	388.22	Joback Method
hvapt	45.00	kJ/mol	395.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35744e+01
Coeff. B	-2.96196e+03
Coeff. C	-1.04429e+02
Temperature range (K), min.	327.35
Temperature range (K), max.	462.89

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C626926&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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/49-698-4/Pentane-1-4-dichloro.pdf

Generated by Cheméo on 2024-04-28 18:04:10.481985301 +0000 UTC m=+16616699.402562612.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.