Pentane, 2,2-dichloro-

Other names: 2,2-Dichloropentane
Inchi: InChI=1S/C5H10Cl2/c1-3-4-5(2,6)7/h3-4H2,1-2H3
InchiKey: MNXVHBFCELLVBA-UHFFFAOYSA-N
Formula: C5H10Cl2
SMILES: CCCC(C)(Cl)Cl
Mol. weight [g/mol]: 141.04
CAS: 34887-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-29.80	kJ/mol	Joback Method
hf	-186.76	kJ/mol	Joback Method
hfus	9.69	kJ/mol	Joback Method
hvap	34.20	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.980		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	831.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	831.00		NIST Webbook
ripol	1043.00		NIST Webbook
tb	401.70	K	NIST Webbook
tb	399.65 ± 2.00	K	NIST Webbook
tc	579.04	K	Joback Method
tf	208.37	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.40	J/mol×K	385.43	Joback Method
cpg	222.52	J/mol×K	546.77	Joback Method

cpg	214.58	J/mol×K	514.50	Joback Method
cpg	206.13	J/mol×K	482.23	Joback Method
cpg	197.13	J/mol×K	449.97	Joback Method
cpg	187.56	J/mol×K	417.70	Joback Method
cpg	229.97	J/mol×K	579.04	Joback Method
dvisc	0.0003821	Pa×s	385.43	Joback Method
dvisc	0.0005124	Pa×s	355.92	Joback Method
dvisc	0.0007246	Pa×s	326.41	Joback Method
dvisc	0.0010979	Pa×s	296.90	Joback Method
dvisc	0.0018231	Pa×s	267.39	Joback Method
dvisc	0.0034334	Pa×s	237.88	Joback Method
dvisc	0.0077359	Pa×s	208.37	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	309.70	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31975e+01
Coeff. B	-2.61861e+03
Coeff. C	-9.64700e+01
Temperature range (K), min.	299.31
Temperature range (K), max.	428.53

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=C34887144&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/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume