

Pentane, 3,3-dichloro-

Other names:	3,3-dichloropentane
Inchi:	InChI=1S/C5H10Cl2/c1-3-5(6,7)4-2/h3-4H2,1-2H3
InchiKey:	MOUDFOLIRVUWKC-UHFFFAOYSA-N
Formula:	C5H10Cl2
SMILES:	CCC(Cl)(Cl)CC
Mol. weight [g/mol]:	141.04
CAS:	21571-91-5

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	820.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
ripol	1074.00		NIST Webbook
tb	404.00 ± 8.00	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/molxK	385.43	Joback Method
cpg	187.56	J/molxK	417.70	Joback Method
cpg	197.13	J/molxK	449.97	Joback Method
cpg	206.13	J/molxK	482.23	Joback Method

cpg	214.58	J/molxK	514.50	Joback Method
cpg	222.52	J/molxK	546.77	Joback Method
cpg	229.97	J/molxK	579.04	Joback Method
dvisc	0.0077359	Paxs	208.37	Joback Method
dvisc	0.0034334	Paxs	237.88	Joback Method
dvisc	0.0018231	Paxs	267.39	Joback Method
dvisc	0.0010979	Paxs	296.90	Joback Method
dvisc	0.0007246	Paxs	326.41	Joback Method
dvisc	0.0005124	Paxs	355.92	Joback Method
dvisc	0.0003821	Paxs	385.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34248e+01
Coeff. B	-2.69568e+03
Coeff. C	-9.78970e+01
Temperature range (K), min.	303.09
Temperature range (K), max.	430.15

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21571915&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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