Benzene, 1,4-dichloro-2-methyl-

Other names:	2,5-Dichlorotoluene
	Toluene, 2,5-dichloro-
Inchi:	InChI=1S/C7H6Cl2/c1-5-4-6(8)2-3-7(5)9/h2-4H,1H3
InchiKey:	KFAKZJUYBOYVKA-UHFFFAOYSA-N
Formula:	C7H6Cl2
SMILES:	Cc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	161.03
CAS:	19398-61-9

Physical Properties

Property code	Value	Unit	Source
gf	77.35	kJ/mol	Joback Method
hf	-5.70	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	43.55	kJ/mol	Joback Method
ie	8.81	eV	NIST Webbook
ie	8.75 ± 0.02	eV	NIST Webbook
log10ws	-3.32		Crippen Method
logp	3.302		Crippen Method
mcvol	110.210	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1098.00		NIST Webbook
tb	471.70	K	NIST Webbook
tc	700.48	K	Joback Method
tf	279.95	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.67	J/mol×K	471.06	Joback Method
cpg	195.96	J/mol×K	509.30	Joback Method
cpg	204.68	J/mol×K	547.53	Joback Method
cpg	212.85	J/mol×K	585.77	Joback Method
cpg	220.49	J/mol×K	624.01	Joback Method
cpg	227.64	J/mol×K	662.24	Joback Method
cpg	234.30	J/mol×K	700.48	Joback Method
dvisc	0.0016666	Pa×s	279.95	Joback Method
dvisc	0.0010588	Pa×s	311.80	Joback Method
dvisc	0.0007317	Pa×s	343.65	Joback Method
dvisc	0.0005384	Pa×s	375.50	Joback Method
dvisc	0.0004156	Pa×s	407.36	Joback Method
dvisc	0.0003331	Pa×s	439.21	Joback Method
dvisc	0.0002751	Pa×s	471.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40370e+01
Coeff. B	-3.75818e+03
Coeff. C	-7.26860e+01
Temperature range (K), min.	346.02
Temperature range (K), max.	503.40

Sources

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

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=C19398619&Units=SI

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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume