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

Other names: 3,4-Dichlorotoluene
Toluene, 3,4-dichloro-
Inchi: InChI=1S/C7H6Cl2/c1-5-2-3-6(8)7(9)4-5/h2-4H,1H3
InchiKey: WYUIWKFIFOJVKW-UHFFFAOYSA-N
Formula: C7H6Cl2
SMILES: Cc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 161.03
CAS: 95-75-0

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	8.85	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	1125.00		NIST Webbook
rinpol	1126.30		NIST Webbook
rinpol	1139.00		NIST Webbook
tb	482.10	K	NIST Webbook
tc	700.48	K	Joback Method
tf	257.90 ± 0.02	K	NIST Webbook
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
hvapt	49.40	kJ/mol	460.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	473.70	K	98.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39535e+01
Coeff. B	-3.79884e+03
Coeff. C	-7.51600e+01
Temperature range (K), min.	353.14
Temperature range (K), max.	514.74

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=C95750&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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume