Benzene, 1,2,4-trichloro-3-methyl-

Other names:	2,3,6-Trichlorotoluene
	Benzene, 1-methyl-2,3,6-trichloro-
	Toluene, 2,3,6-trichloro-
Inchi:	InChI=1S/C7H5Cl3/c1-4-5(8)2-3-6(9)7(4)10/h2-3H,1H3
InchiKey:	UZYYBZNZSSNYSA-UHFFFAOYSA-N
Formula:	C7H5Cl3
SMILES:	Cc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	195.47
CAS:	2077-46-5

Physical Properties

Property code	Value	Unit	Source
gf	55.79	kJ/mol	Joback Method
hf	-32.91	kJ/mol	Joback Method
hfus	19.35	kJ/mol	Joback Method
hvap	48.59	kJ/mol	Joback Method
ie	8.85	eV	NIST Webbook
log10ws	-4.00		Crippen Method
logp	3.955		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	513.47	K	Joback Method
tc	749.79	K	Joback Method
tf	322.39	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.42	J/mol×K	749.79	Joback Method
cpg	243.55	J/mol×K	710.40	Joback Method
cpg	237.23	J/mol×K	671.02	Joback Method
cpg	230.46	J/mol×K	631.63	Joback Method
cpg	223.21	J/mol×K	592.24	Joback Method

cpg	215.47	J/mol×K	552.86	Joback Method
cpg	207.21	J/mol×K	513.47	Joback Method
dvisc	0.0013398	Pa×s	322.39	Joback Method
dvisc	0.0002778	Pa×s	513.47	Joback Method
dvisc	0.0003311	Pa×s	481.62	Joback Method
dvisc	0.0004045	Pa×s	449.78	Joback Method
dvisc	0.0005096	Pa×s	417.93	Joback Method
dvisc	0.0006669	Pa×s	386.08	Joback Method
dvisc	0.0009161	Pa×s	354.24	Joback Method
hvapt	62.20	kJ/mol	446.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25104e+01
Coeff. B	-3.37735e+03
Coeff. C	-7.56050e+01
Temperature range (K), min.	351.92
Temperature range (K), max.	544.75

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2077465&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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