Benzene, 1,3-dichloro-5-methyl-

Other names:	3,5-Dichlorotoluene
	Toluene, 3,5-dichloro-
Inchi:	InChI=1S/C7H6Cl2/c1-5-2-6(8)4-7(9)3-5/h2-4H,1H3
InchiKey:	RYMMNSVHOKXTNN-UHFFFAOYSA-N
Formula:	C7H6Cl2
SMILES:	Cc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	161.03
CAS:	25186-47-4

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	9.99 ± 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
tb	474.70	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	227.64	J/mol×K	662.24	Joback Method
cpg	220.49	J/mol×K	624.01	Joback Method
cpg	212.85	J/mol×K	585.77	Joback Method
cpg	204.68	J/mol×K	547.53	Joback Method
cpg	195.96	J/mol×K	509.30	Joback Method

cpg	234.30	J/mol×K	700.48	Joback Method
dvisc	0.0002751	Pa×s	471.06	Joback Method
dvisc	0.0003331	Pa×s	439.21	Joback Method
dvisc	0.0004156	Pa×s	407.36	Joback Method
dvisc	0.0005384	Pa×s	375.50	Joback Method
dvisc	0.0007317	Pa×s	343.65	Joback Method
dvisc	0.0010588	Pa×s	311.80	Joback Method
dvisc	0.0016666	Pa×s	279.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39306e+01
Coeff. B	-3.73978e+03
Coeff. C	-7.31030e+01
Temperature range (K), min.	347.22
Temperature range (K), max.	507.00

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=C25186474&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume