Benzene, 1,3-dichloro-2-methyl-

Other names:	1,3-dichloro-2-methylbenzene
	2,6-Dichlorotoluene
	2,6-dichloro-1-methylbenzene
	Toluene, 2,6-dichloro-
Inchi:	InChI=1S/C7H6Cl2/c1-5-6(8)3-2-4-7(5)9/h2-4H,1H3
InchiKey:	DMEDNTFWIHCBRK-UHFFFAOYSA-N
Formula:	C7H6Cl2
SMILES:	Cc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	161.03
CAS:	118-69-4

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
log10ws	-3.32		Crippen Method
logp	3.302		Crippen Method
mcvol	110.210	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1104.00		NIST Webbook
tb	472.70	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
hfust	10.70	kJ/mol	272.00	NIST Webbook
pvap	0.03	kPa	274.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.04	kPa	276.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.05	kPa	278.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.06	kPa	280.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.07	kPa	282.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.08	kPa	284.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.11	kPa	288.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

pvap	0.13	kPa	291.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.15	kPa	293.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.19	kPa	296.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.22	kPa	298.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.27	kPa	301.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.35	kPa	305.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38109e+01
Coeff. B	-3.68225e+03
Coeff. C	-7.21300e+01
Temperature range (K), min.	344.42
Temperature range (K), max.	505.37

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes:	https://www.doi.org/10.1016/j.fluid.2014.07.029
Liquid–Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous–Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
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=C118694&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

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
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume