

# Benzene, 2,4-dichloro-1-(chloromethyl)-

<b>Other names:</b>	2,4-Dichloro-1-(chloromethyl)benzene 2,4-Dichlorobenzyl chloride Toluene, «alpha»2,4-trichloro- Toluene, Â«alphaÂ»2,4-trichloro- «alpha»,2,4-Trichlorotoluene Â«alphaÂ»,2,4-Trichlorotoluene
<b>Inchi:</b>	InChI=1S/C7H5Cl3/c8-4-5-1-2-6(9)3-7(5)10/h1-3H,4H2
<b>InchiKey:</b>	IRSVDHPYXFL LDS-UHFFFAOYSA-N
<b>Formula:</b>	C7H5Cl3
<b>SMILES:</b>	ClCc1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	195.47
<b>CAS:</b>	94-99-5

## Physical Properties

Property code	Value	Unit	Source
gf	65.42	kJ/mol	Joback Method
hf	-21.44	kJ/mol	Joback Method
hfus	19.74	kJ/mol	Joback Method
hvap	47.93	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.732		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1314.50		NIST Webbook
tb	521.20	K	NIST Webbook
tc	743.54	K	Joback Method
tf	271.00 ± 0.02	K	NIST Webbook
vc	0.467	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.62	J/molxK	743.54	Joback Method
cpg	245.65	J/molxK	704.37	Joback Method

cpg	239.19	J/molxK	665.19	Joback Method
cpg	232.23	J/molxK	626.02	Joback Method
cpg	224.73	J/molxK	586.84	Joback Method
cpg	216.67	J/molxK	547.67	Joback Method
cpg	208.02	J/molxK	508.49	Joback Method
dvisc	0.0017070	Paxs	309.87	Joback Method
dvisc	0.0002870	Paxs	508.49	Joback Method
dvisc	0.0003484	Paxs	475.39	Joback Method
dvisc	0.0004353	Paxs	442.28	Joback Method
dvisc	0.0005638	Paxs	409.18	Joback Method
dvisc	0.0007643	Paxs	376.08	Joback Method
dvisc	0.0010988	Paxs	342.97	Joback Method
hvapt	54.60	kJ/mol	495.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38187e+01
Coeff. B	-4.00371e+03
Coeff. C	-8.60300e+01
Temperature range (K), min.	381.92
Temperature range (K), max.	556.66

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C94995&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94995&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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