

# Benzene, 1-(chloromethyl)-2-methyl-

<b>Other names:</b>	1-(Chloromethyl)-2-methylbenzene 2-(Chloromethyl)toluene 2-Methylbenzyl chloride o-(Chloromethyl)toluene o-Methylbenzyl chloride o-Xylene, «alpha»-chloro- o-Xylene, Â«alphaÂ»-chloro- o-Xylyl chloride o-Xylyl-«alpha»-chloride o-Xylyl-Â«alphaÂ»-chloride «alpha»-Chloro-o-xylene «alpha»-Chloro-ortho-xylene «omega»-Chloro-o-xylene Â«alphaÂ»-Chloro-o-xylene Â«alphaÂ»-Chloro-ortho-xylene Â«omegaÂ»-Chloro-o-xylene
<b>Inchi:</b>	InChI=1S/C8H9Cl/c1-7-4-2-3-5-8(7)6-9/h2-5H,6H2,1H3
<b>InchiKey:</b>	VQRBXYYBBGHOGFT-UHFFFAOYSA-N
<b>Formula:</b>	C8H9Cl
<b>SMILES:</b>	Cc1cccc1CCl
<b>Mol. weight [g/mol]:</b>	140.61
<b>CAS:</b>	552-45-4

## Physical Properties

Property code	Value	Unit	Source
gf	107.33	kJ/mol	Joback Method
hf	0.87	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	40.73	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.734		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1105.00		NIST Webbook
tb	471.20	K	NIST Webbook
tc	669.70	K	Joback Method

tf	248.78	K	Joback Method
vc	0.424	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.26	J/mol×K	451.53	Joback Method
cpg	254.26	J/mol×K	633.34	Joback Method
cpg	245.12	J/mol×K	596.98	Joback Method
cpg	235.38	J/mol×K	560.62	Joback Method
cpg	225.00	J/mol×K	524.25	Joback Method
cpg	213.97	J/mol×K	487.89	Joback Method
cpg	262.83	J/mol×K	669.70	Joback Method
dvisc	0.0002545	Paxs	451.53	Joback Method
dvisc	0.0003165	Paxs	417.74	Joback Method
dvisc	0.0004090	Paxs	383.95	Joback Method
dvisc	0.0005554	Paxs	350.15	Joback Method
dvisc	0.0008051	Paxs	316.36	Joback Method
dvisc	0.0012755	Paxs	282.57	Joback Method
dvisc	0.0022898	Paxs	248.78	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41938e+01
Coeff. B	-3.82130e+03
Coeff. C	-7.21300e+01
Temperature range (K), min.	346.92
Temperature range (K), max.	502.34

## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C552454&Units=SI>

**The Yaws Handbook of Vapor**

**Pressure:**

**Crippen Method:**

**Crippen Method:**

**Joback Method:**

**McGowan Method:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

## 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>hvap:</b>	Enthalpy of vaporization at standard conditions
<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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