

# 1,2,4-Trimethyl-5,6-bis(chloromethyl)benzene

<b>Inchi:</b>	InChI=1S/C11H14Cl2/c1-7-4-8(2)10(5-12)11(6-13)9(7)3/h4H,5-6H2,1-3H3
<b>InchiKey:</b>	CJTRVCWKFQQWJL-UHFFFAOYSA-N
<b>Formula:</b>	C11H14Cl2
<b>SMILES:</b>	<chem>Cc1cc(C)c(CCl)c(CCl)c1C</chem>
<b>Mol. weight [g/mol]:</b>	217.13

## Physical Properties

Property code	Value	Unit	Source
gf	91.77	kJ/mol	Joback Method
hf	-111.20	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	53.77	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.089		Crippen Method
mcvol	166.570	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1658.00		NIST Webbook
tb	572.54	K	Joback Method
tc	788.86	K	Joback Method
tf	350.07	K	Joback Method
vc	0.641	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.71	J/molxK	572.54	Joback Method
cpg	369.87	J/molxK	608.59	Joback Method
cpg	382.35	J/molxK	644.65	Joback Method
cpg	394.17	J/molxK	680.70	Joback Method
cpg	405.35	J/molxK	716.75	Joback Method
cpg	415.89	J/molxK	752.80	Joback Method
cpg	425.82	J/molxK	788.86	Joback Method
dvisc	0.0011000	Paxs	350.07	Joback Method
dvisc	0.0007263	Paxs	387.15	Joback Method

dvisc	0.0005157	Paxs	424.23	Joback Method
dvisc	0.0003868	Paxs	461.31	Joback Method
dvisc	0.0003029	Paxs	498.38	Joback Method
dvisc	0.0002453	Paxs	535.46	Joback Method
dvisc	0.0002042	Paxs	572.54	Joback Method

## Sources

<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>
<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=R520139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R520139&amp;Units=SI</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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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