

# Anisole, 2,4-bis(chloromethyl)-

<b>Inchi:</b>	InChI=1S/C9H10Cl2O/c1-12-9-3-2-7(5-10)4-8(9)6-11/h2-4H,5-6H2,1H3
<b>InchiKey:</b>	ZBQXEAI GIXABOB-UHFFFAOYSA-N
<b>Formula:</b>	C9H10Cl2O
<b>SMILES:</b>	COc1ccc(CCl)cc1CCl
<b>Mol. weight [g/mol]:</b>	205.08
<b>CAS:</b>	25445-34-5

## Physical Properties

Property code	Value	Unit	Source
gf	-10.81	kJ/mol	Joback Method
hf	-179.20	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.173		Crippen Method
mcvol	144.260	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	539.24	K	Joback Method
tc	758.44	K	Joback Method
tf	324.72	K	Joback Method
vc	0.547	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.67	J/molxK	539.24	Joback Method
cpg	302.27	J/molxK	575.77	Joback Method
cpg	313.24	J/molxK	612.31	Joback Method
cpg	323.60	J/molxK	648.84	Joback Method
cpg	333.37	J/molxK	685.37	Joback Method
cpg	342.54	J/molxK	721.91	Joback Method
cpg	351.13	J/molxK	758.44	Joback Method
dvisc	0.0013666	Paxs	324.72	Joback Method
dvisc	0.0008503	Paxs	360.47	Joback Method

dvisc	0.0005763	Paxs	396.23	Joback Method
dvisc	0.0004166	Paxs	431.98	Joback Method
dvisc	0.0003165	Paxs	467.73	Joback Method
dvisc	0.0002500	Paxs	503.49	Joback Method
dvisc	0.0002037	Paxs	539.24	Joback Method

## Sources

<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=C25445345&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25445345&amp;Units=SI</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>

## 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>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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