

# 2-Allyl-4-chlorophenyl allyl ether

<b>Inchi:</b>	InChI=1S/C12H13ClO/c1-3-5-10-9-11(13)6-7-12(10)14-8-4-2/h3-4,6-7,9H,1-2,5,8H2
<b>InchiKey:</b>	BWKRYENOKBVWNT-UHFFFAOYSA-N
<b>Formula:</b>	C12H13ClO
<b>SMILES:</b>	C=CCOc1ccc(Cl)cc1CC=C
<b>Mol. weight [g/mol]:</b>	208.68
<b>CAS:</b>	51496-26-5

## Physical Properties

Property code	Value	Unit	Source
gf	202.06	kJ/mol	Joback Method
hf	25.48	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	51.36	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.633		Crippen Method
mvol	165.690	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
tb	563.81	K	Joback Method
tc	776.70	K	Joback Method
tf	325.09	K	Joback Method
vc	0.628	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.30	J/molxK	563.81	Joback Method
cpg	376.04	J/molxK	599.29	Joback Method
cpg	389.01	J/molxK	634.77	Joback Method
cpg	401.23	J/molxK	670.26	Joback Method
cpg	412.73	J/molxK	705.74	Joback Method
cpg	423.52	J/molxK	741.22	Joback Method
cpg	433.65	J/molxK	776.70	Joback Method
dvisc	0.0012666	Paxs	325.09	Joback Method
dvisc	0.0007571	Paxs	364.88	Joback Method

dvisc	0.0005007	Paxs	404.66	Joback Method
dvisc	0.0003566	Paxs	444.45	Joback Method
dvisc	0.0002685	Paxs	484.24	Joback Method
dvisc	0.0002111	Paxs	524.02	Joback Method
dvisc	0.0001717	Paxs	563.81	Joback Method

## 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=C51496265&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51496265&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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>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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