

# Allyl-2,5-dichlorophenyl ether

<b>Inchi:</b>	InChI=1S/C9H8Cl2O/c1-2-5-12-9-6-7(10)3-4-8(9)11/h2-4,6H,1,5H2
<b>InchiKey:</b>	URPPDFSAIGMPMJ-UHFFFAOYSA-N
<b>Formula:</b>	C9H8Cl2O
<b>SMILES:</b>	C=CCOc1cc(Cl)ccc1Cl
<b>Mol. weight [g/mol]:</b>	203.06
<b>CAS:</b>	116435-13-3

## Physical Properties

Property code	Value	Unit	Source
gf	77.03	kJ/mol	Joback Method
hf	-53.77	kJ/mol	Joback Method
hfus	20.63	kJ/mol	Joback Method
hvap	49.74	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.558		Crippen Method
mcvol	139.960	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	535.92	K	Joback Method
tc	759.97	K	Joback Method
tf	322.96	K	Joback Method
vc	0.528	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.97	J/molxK	535.92	Joback Method
cpg	282.77	J/molxK	573.26	Joback Method
cpg	292.95	J/molxK	610.60	Joback Method
cpg	302.51	J/molxK	647.95	Joback Method
cpg	311.48	J/molxK	685.29	Joback Method
cpg	319.87	J/molxK	722.63	Joback Method
cpg	327.69	J/molxK	759.97	Joback Method
dvisc	0.0013018	Paxs	322.96	Joback Method
dvisc	0.0008248	Paxs	358.45	Joback Method

dvisc	0.0005674	Paxs	393.95	Joback Method
dvisc	0.0004152	Paxs	429.44	Joback Method
dvisc	0.0003187	Paxs	464.93	Joback Method
dvisc	0.0002540	Paxs	500.43	Joback Method
dvisc	0.0002086	Paxs	535.92	Joback Method

## Sources

<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=C116435133&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116435133&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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