

# P-isopropylphenyl allyl ether

<b>Inchi:</b>	InChI=1S/C12H16O/c1-4-9-13-12-7-5-11(6-8-12)10(2)3/h4-8,10H,1,9H2,2-3H3
<b>InchiKey:</b>	QVGYGYMFMUBSHD-UHFFFAOYSA-N
<b>Formula:</b>	C12H16O
<b>SMILES:</b>	<chem>C=CCOc1ccc(C(C)C)cc1</chem>
<b>Mol. weight [g/mol]:</b>	176.25
<b>CAS:</b>	71029-37-3

## Physical Properties

Property code	Value	Unit	Source
gf	133.34	kJ/mol	Joback Method
hf	-78.02	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	46.60	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.375		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	524.28	K	Joback Method
tc	731.65	K	Joback Method
tf	269.41	K	Joback Method
vc	0.593	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.69	J/molxK	524.28	Joback Method
cpg	369.61	J/molxK	558.84	Joback Method
cpg	384.69	J/molxK	593.40	Joback Method
cpg	398.97	J/molxK	627.97	Joback Method
cpg	412.45	J/molxK	662.53	Joback Method
cpg	425.16	J/molxK	697.09	Joback Method
cpg	437.13	J/molxK	731.65	Joback Method
dvisc	0.0024807	Paxs	269.41	Joback Method
dvisc	0.0011520	Paxs	311.89	Joback Method

dvisc	0.0006430	Paxs	354.37	Joback Method
dvisc	0.0004066	Paxs	396.85	Joback Method
dvisc	0.0002809	Paxs	439.32	Joback Method
dvisc	0.0002072	Paxs	481.80	Joback Method
dvisc	0.0001605	Paxs	524.28	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=C71029373&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C71029373&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>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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