

# trans-2-Methoxy-4-methyl-2-pentene

<b>Inchi:</b>	InChI=1S/C7H14O/c1-6(2)5-7(3)8-4/h5-6H,1-4H3/b7-5+
<b>InchiKey:</b>	VUVRRRJAGXVQQZ-FNORWQNLSA-N
<b>Formula:</b>	C7H14O
<b>SMILES:</b>	COC(C)=CC(C)C
<b>Mol. weight [g/mol]:</b>	114.19
<b>CAS:</b>	53119-72-5

## Physical Properties

Property code	Value	Unit	Source
gf	-27.71	kJ/mol	Joback Method
hf	-217.88	kJ/mol	Joback Method
hfus	10.44	kJ/mol	Joback Method
hvap	33.24	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.193		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
tb	385.58	K	Joback Method
tc	566.06	K	Joback Method
tf	156.84	K	Joback Method
vc	0.420	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.89	J/mol×K	385.58	Joback Method
cpg	215.76	J/mol×K	415.66	Joback Method
cpg	227.17	J/mol×K	445.74	Joback Method
cpg	238.14	J/mol×K	475.82	Joback Method
cpg	248.67	J/mol×K	505.90	Joback Method
cpg	258.77	J/mol×K	535.98	Joback Method
cpg	268.46	J/mol×K	566.06	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=C53119725&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53119725&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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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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