

# Isobutyl methyl carbonate

<b>Inchi:</b>	InChI=1S/C6H12O3/c1-5(2)4-9-6(7)8-3/h5H,4H2,1-3H3
<b>InchiKey:</b>	PDOXCFPUGNQQSW-UHFFFAOYSA-N
<b>Formula:</b>	C6H12O3
<b>SMILES:</b>	COC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	132.16

## Physical Properties

Property code	Value	Unit	Source
gf	-341.72	kJ/mol	Joback Method
hf	-549.47	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	40.13	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.425		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpola	857.30		NIST Webbook
tb	434.95	K	Joback Method
tc	616.32	K	Joback Method
tf	236.77	K	Joback Method
vc	0.407	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.96	J/molxK	434.95	Joback Method
cpg	231.96	J/molxK	465.18	Joback Method
cpg	241.69	J/molxK	495.41	Joback Method
cpg	251.15	J/molxK	525.64	Joback Method
cpg	260.32	J/molxK	555.87	Joback Method
cpg	269.18	J/molxK	586.09	Joback Method
cpg	277.74	J/molxK	616.32	Joback Method
dvisc	0.0034104	Paxs	236.77	Joback Method
dvisc	0.0016505	Paxs	269.80	Joback Method

dvisc	0.0009358	Paxs	302.83	Joback Method
dvisc	0.0005932	Paxs	335.86	Joback Method
dvisc	0.0004081	Paxs	368.89	Joback Method
dvisc	0.0002985	Paxs	401.92	Joback Method
dvisc	0.0002290	Paxs	434.95	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=U333939&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333939&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>
<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>rinpol:</b>	Non-polar retention indices
<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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