

# Propane, 1,1-dimethoxy-2-methyl-

<b>Other names:</b>	Isobutylaldehyde dimethyl acetal Isobutyraldehyde dimethylacetal 1,1-Dimethoxy-2-methylpropane Propane, 2-methyl, 1,1-dimethoxy Isobutanal, dimethylacetal
<b>Inchi:</b>	InChI=1S/C6H14O2/c1-5(2)6(7-3)8-4/h5-6H,1-4H3
<b>InchiKey:</b>	YINGOXPFQFTXIX-UHFFFAOYSA-N
<b>Formula:</b>	C6H14O2
<b>SMILES:</b>	COC(OC)C(C)C
<b>Mol. weight [g/mol]:</b>	118.17
<b>CAS:</b>	41632-89-7

## Physical Properties

Property code	Value	Unit	Source
gf	-215.24	kJ/mol	Joback Method
hf	-442.17	kJ/mol	Joback Method
hfus	6.63	kJ/mol	Joback Method
hvap	32.99	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	1.261		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	733.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	701.00		NIST Webbook
tb	380.64	K	Joback Method
tc	553.72	K	Joback Method
tf	184.10 ± 0.60	K	NIST Webbook
vc	0.396	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.51	J/mol×K	380.64	Joback Method
cpg	215.09	J/mol×K	409.49	Joback Method
cpg	225.43	J/mol×K	438.33	Joback Method
cpg	235.51	J/mol×K	467.18	Joback Method
cpg	245.33	J/mol×K	496.03	Joback Method
cpg	254.88	J/mol×K	524.87	Joback Method
cpg	264.15	J/mol×K	553.72	Joback Method
dvisc	0.0086655	Paxs	171.84	Joback Method
dvisc	0.0026859	Paxs	206.64	Joback Method
dvisc	0.0011669	Paxs	241.44	Joback Method
dvisc	0.0006254	Paxs	276.24	Joback Method
dvisc	0.0003854	Paxs	311.04	Joback Method
dvisc	0.0002618	Paxs	345.84	Joback Method
dvisc	0.0001909	Paxs	380.64	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C41632897&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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