

# 2,2-Dimethoxybutane

<b>Other names:</b>	2-butanone, dimethyl acetal Butane, 2,2-dimethoxy butane, 2,2-dimethoxy-
<b>Inchi:</b>	InChI=1S/C6H14O2/c1-5-6(2,7-3)8-4/h5H2,1-4H3
<b>InchiKey:</b>	OXQHJIGWZNIQDS-UHFFFAOYSA-N
<b>Formula:</b>	C6H14O2
<b>SMILES:</b>	CCC(C)(OC)OC
<b>Mol. weight [g/mol]:</b>	118.17
<b>CAS:</b>	3453-99-4

## Physical Properties

Property code	Value	Unit	Source
gf	-207.52	kJ/mol	Joback Method
hf	-440.36	kJ/mol	Joback Method
hfus	6.26	kJ/mol	Joback Method
hvap	32.47	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.405		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinsol	740.00		NIST Webbook
tb	378.29	K	Joback Method
tc	554.52	K	Joback Method
tf	204.26	K	Joback Method
vc	0.397	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.08	J/molxK	554.52	Joback Method
cpg	205.93	J/molxK	378.29	Joback Method
cpg	217.24	J/molxK	407.66	Joback Method
cpg	228.17	J/molxK	437.03	Joback Method
cpg	238.72	J/molxK	466.41	Joback Method

cpg	248.88	J/mol×K	495.78	Joback Method
cpg	258.67	J/mol×K	525.15	Joback Method
dvisc	0.0002307	Paxs	378.29	Joback Method
dvisc	0.0049367	Paxs	204.26	Joback Method
dvisc	0.0021570	Paxs	233.26	Joback Method
dvisc	0.0011319	Paxs	262.27	Joback Method
dvisc	0.0006753	Paxs	291.27	Joback Method
dvisc	0.0004425	Paxs	320.28	Joback Method
dvisc	0.0003110	Paxs	349.28	Joback Method
hfust	9.32	kJ/mol	174.00	NIST Webbook

## Sources

**McGowan Method:**

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

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3453994&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

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

**Excess Molar Enthalpies for the Binary Systems of Benzene or Cyclohexane**

**with 1,1-Diethoxyethane at 323.15 K or with 2,2-Dimethoxybutane at 303.15 K and Infinite Dilution Activity**

<https://www.doi.org/10.1021/je020195l>

**Coefficients in 1,1-Diethoxyethane:**

[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>hfust:</b>	Enthalpy of fusion at a given temperature
<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>mvol:</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

Latest version available from:

<https://www.cheméo.com/cid/62-345-0/2-2-Dimethoxybutane.pdf>

Generated by Cheméo on 2024-04-19 20:47:04.126186781 +0000 UTC m=+15848873.046764093.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.