

2,2-Dimethoxybutane

Other names:	2-butanone, dimethyl acetal Butane, 2,2-dimethoxy butane, 2,2-dimethoxy-
Inchi:	InChI=1S/C6H14O2/c1-5-6(2,7-3)8-4/h5H2,1-4H3
InchiKey:	OXQHJIGWZNIQDS-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CCC(C)(OC)OC
Mol. weight [g/mol]:	118.17
CAS:	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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.08	J/mol×K	554.52	Joback Method
cpg	258.67	J/mol×K	525.15	Joback Method
cpg	248.88	J/mol×K	495.78	Joback Method
cpg	238.72	J/mol×K	466.41	Joback Method
cpg	228.17	J/mol×K	437.03	Joback Method

cpg	217.24	J/mol×K	407.66	Joback Method
cpg	205.93	J/mol×K	378.29	Joback Method
dvisc	0.0049367	Pa×s	204.26	Joback Method
dvisc	0.0002307	Pa×s	378.29	Joback Method
dvisc	0.0003110	Pa×s	349.28	Joback Method
dvisc	0.0004425	Pa×s	320.28	Joback Method
dvisc	0.0006753	Pa×s	291.27	Joback Method
dvisc	0.0011319	Pa×s	262.27	Joback Method
dvisc	0.0021570	Pa×s	233.26	Joback Method
hfust	9.32	kJ/mol	174.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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/ci990307l
Crippen Method:	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 Coefficients in 1,1-Diethoxyethane: <https://www.doi.org/10.1021/je020195l>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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