

2-Propanone, 1,1-dimethoxy-

Other names:	Pyruvic aldehyde dimethyl acetal Methylglyoxal dimethyl acetal 1,1-Dimethoxyacetone Pyruvaldehyde-1,1-(dimethyl acetal) Dimethoxymethyl methyl ketone Pyruvaldehyde dimethyl acetal Pyruvaldehyde, 1-(dimethyl acetal) 1,1-Dimethoxy-2-propanone NSC 50127
Inchi:	InChI=1S/C5H10O3/c1-4(6)5(7-2)8-3/h5H,1-3H3
InchiKey:	ULVSHNOGEVXRDR-UHFFFAOYSA-N
Formula:	C5H10O3
SMILES:	COC(OC)C(C)=O
Mol. weight [g/mol]:	118.13
CAS:	6342-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-350.14	kJ/mol	Joback Method
hf	-528.83	kJ/mol	Joback Method
hfus	9.16	kJ/mol	Joback Method
hvap	37.90	kJ/mol	Joback Method
log10ws	0.02		Crippen Method
logp	0.194		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	418.20	K	NIST Webbook
tc	594.82	K	Joback Method
tf	225.50	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	184.38	J/mol×K	412.07	Joback Method
cpg	192.98	J/mol×K	442.53	Joback Method
cpg	201.39	J/mol×K	472.99	Joback Method
cpg	209.59	J/mol×K	503.45	Joback Method
cpg	217.57	J/mol×K	533.90	Joback Method
cpg	225.32	J/mol×K	564.36	Joback Method
cpg	232.83	J/mol×K	594.82	Joback Method
dvisc	0.0032948	Pa×s	225.50	Joback Method
dvisc	0.0016301	Pa×s	256.60	Joback Method
dvisc	0.0009390	Pa×s	287.69	Joback Method
dvisc	0.0006024	Pa×s	318.78	Joback Method
dvisc	0.0004181	Pa×s	349.88	Joback Method
dvisc	0.0003081	Pa×s	380.98	Joback Method
dvisc	0.0002377	Pa×s	412.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C6342569&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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