2-Propanone, 1,1-diethoxy-

Other names: Pyruvaldehyde, 1-(diethyl acetal)
1,1-Diethoxyacetone
Inchi: InChI=1S/C7H14O3/c1-4-9-7(6(3)8)10-5-2/h7H,4-5H2,1-3H3
InchiKey: SDMOBEHDSJVJHU-UHFFFAOYSA-N
Formula: C7H14O3
SMILES: CCOC(OCC)C(C)=O
Mol. weight [g/mol]: 146.18
CAS: 5774-26-5

Physical Properties

Property code	Value	Unit	Source
gf	-333.30	kJ/mol	Joback Method
hf	-570.11	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	42.35	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.974		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
ripol	1252.00		NIST Webbook
tb	457.83	K	Joback Method
tc	637.68	K	Joback Method
tf	248.04	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.88	J/mol×K	457.83	Joback Method
cpg	273.14	J/mol×K	487.81	Joback Method
cpg	284.07	J/mol×K	517.78	Joback Method
cpg	294.65	J/mol×K	547.76	Joback Method
cpg	304.87	J/mol×K	577.73	Joback Method
cpg	314.74	J/mol×K	607.71	Joback Method

cpg	324.24	J/mol×K	637.68	Joback Method
dvisc	0.0034521	Pa×s	248.04	Joback Method
dvisc	0.0016371	Pa×s	283.00	Joback Method
dvisc	0.0009148	Pa×s	317.97	Joback Method
dvisc	0.0005737	Pa×s	352.94	Joback Method
dvisc	0.0003913	Pa×s	387.90	Joback Method
dvisc	0.0002844	Pa×s	422.87	Joback Method
dvisc	0.0002170	Pa×s	457.83	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=C5774265&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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