

3-Pentanone, 1,5-dimethoxy-

Other names:	1,5-Dimethoxy-3-pentanone
Inchi:	InChI=1S/C7H14O3/c1-9-5-3-7(8)4-6-10-2/h3-6H2,1-2H3
InchiKey:	KPAJOFKZGBPVO-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	COCCC(=O)CCOC
Mol. weight [g/mol]:	146.18
CAS:	53005-18-8

Physical Properties

Property code	Value	Unit	Source
gf	-330.86	kJ/mol	Joback Method
hf	-564.83	kJ/mol	Joback Method
hfus	17.86	kJ/mol	Joback Method
hvap	42.74	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.629		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
ripol	2248.00		NIST Webbook
ripol	2248.00		NIST Webbook
tb	458.27	K	Joback Method
tc	634.29	K	Joback Method
tf	263.04	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.73	J/molxK	458.27	Joback Method
cpg	272.68	J/molxK	487.61	Joback Method
cpg	283.31	J/molxK	516.94	Joback Method
cpg	293.62	J/molxK	546.28	Joback Method
cpg	303.59	J/molxK	575.61	Joback Method
cpg	313.23	J/molxK	604.95	Joback Method

cpg	322.52	J/mol×K	634.29	Joback Method
dvisc	0.0024226	Paxs	263.04	Joback Method
dvisc	0.0013150	Paxs	295.58	Joback Method
dvisc	0.0008058	Paxs	328.12	Joback Method
dvisc	0.0005394	Paxs	360.65	Joback Method
dvisc	0.0003858	Paxs	393.19	Joback Method
dvisc	0.0002905	Paxs	425.73	Joback Method
dvisc	0.0002277	Paxs	458.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53005188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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