2-Butanone, 4,4-dimethoxy-

Other names:	Acetoacetaldehyde, 1-(dimethyl acetal)
	«beta»-Oxobutyraldehyde dimethyl acetal
	Acetoacetaldehyde dimethyl acetal
	Acetylacetaldehyde dimethyl acetal
	1,1-Dimethoxy-3-butanone
	3-Ketobutyraldehyde dimethylacetal
	3-Oxobutyraldehyde dimethyl acetal
	4,4-Dimethoxy-2-butanone
	Acetylacetaldehyddimethylacetal
	Formylacetone dimethyl acetal
	3-Oxobutyraldehyde 1-(dimethylacetal)
	NSC 21538
	NSC 59721
	4,4-dimethoxybutanone
Inchi:	InChI=1S/C6H12O3/c1-5(7)4-6(8-2)9-3/h6H,4H2,1-3H3
InchiKey:	PJCCSZUMZMCWSX-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	COC(CC(C)=O)OC
Mol. weight [g/mol]:	132.16
CAS:	5436-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-341.72	kJ/mol	Joback Method
hf	-549.47	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	40.13	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.584		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	855.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	855.00		NIST Webbook
tb	434.95	K	Joback Method
tc	616.32	K	Joback Method
tf	236.77	K	Joback Method

vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.96	J/mol×K	434.95	Joback Method
cpg	269.18	J/mol×K	586.09	Joback Method
cpg	260.32	J/mol×K	555.87	Joback Method
cpg	251.15	J/mol×K	525.64	Joback Method
cpg	241.69	J/mol×K	495.41	Joback Method
cpg	231.96	J/mol×K	465.18	Joback Method
cpg	277.74	J/mol×K	616.32	Joback Method
dvisc	0.0002290	Pa×s	434.95	Joback Method
dvisc	0.0002985	Pa×s	401.92	Joback Method
dvisc	0.0004081	Pa×s	368.89	Joback Method
dvisc	0.0005932	Pa×s	335.86	Joback Method
dvisc	0.0009358	Pa×s	302.83	Joback Method
dvisc	0.0016505	Pa×s	269.80	Joback Method
dvisc	0.0034104	Pa×s	236.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.70	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5436215&Units=SI

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume