3,3-Dimethoxy-2-butanone

Inchi:	InChI=1S/C6H12O3/c1-5(7)6(2,8-3)9-4/h1-4H3
InchiKey:	UFQBSPGKRRSATO-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	COC(C)(OC)C(C)=O
Mol. weight [g/mol]:	132.16
CAS:	21983-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-336.44	kJ/mol	Joback Method
hf	-552.94	kJ/mol	Joback Method
hfus	7.86	kJ/mol	Joback Method
hvap	39.22	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.584		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	418.70	K	NIST Webbook
tc	621.06	K	Joback Method
tf	254.19	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.41	J/mol×K	432.16	Joback Method
cpg	235.24	J/mol×K	463.64	Joback Method
cpg	245.64	J/mol×K	495.13	Joback Method
cpg	255.63	J/mol×K	526.61	Joback Method
cpg	265.19	J/mol×K	558.09	Joback Method
cpg	274.33	J/mol×K	589.58	Joback Method
cpg	283.05	J/mol×K	621.06	Joback Method
dvisc	0.0033807	Pa×s	254.19	Joback Method
dvisc	0.0017467	Pa×s	283.85	Joback Method

dvisc	0.0010226	Pa×s	313.51	Joback Method
dvisc	0.0006567	Pa×s	343.17	Joback Method
dvisc	0.0004525	Pa×s	372.84	Joback Method
dvisc	0.0003294	Pa×s	402.50	Joback Method
dvisc	0.0002505	Pa×s	432.16	Joback Method

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=C21983722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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