tert-C4H9C(O)OCH(CH3)2

Other names:	2,2-Dimethylpropionic acid, isopropyl ester
	iso-Propyl pivalate
	Propanoic acid, 2,2-dimethyl, 1-methylethyl ester
Inchi:	InChI=1S/C8H16O2/c1-6(2)10-7(9)8(3,4)5/h6H,1-5H3
InchiKey:	PMFKTHJAJBPRNM-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CC(C)OC(=O)C(C)(C)C
Mol. weight [g/mol]:	144.21
CAS:	5129-36-2

Physical Properties

Property code	Value	Unit	Source
gf	-217.04	kJ/mol	Joback Method
hf	-467.28	kJ/mol	Joback Method
hfus	8.33	kJ/mol	Joback Method
hvap	4828.00	kJ/mol	NIST Webbook
log10ws	-1.90		Crippen Method
logp	1.984		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	813.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	946.00		NIST Webbook
ripol	946.00		NIST Webbook
tb	401.00 ± 3.00	K	NIST Webbook
tc	645.31	K	Joback Method
tf	239.50	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.43	J/mol×K	455.06	Joback Method
cpg	345.10	J/mol×K	613.60	Joback Method
cpg	333.80	J/mol×K	581.89	Joback Method
cpg	321.89	J/mol×K	550.18	Joback Method
cpg	309.37	J/mol×K	518.48	Joback Method
cpg	296.22	J/mol×K	486.77	Joback Method
cpg	355.83	J/mol×K	645.31	Joback Method
dvisc	0.0002462	Pa×s	455.06	Joback Method
dvisc	0.0003399	Pa×s	419.13	Joback Method
dvisc	0.0004982	Pa×s	383.21	Joback Method
dvisc	0.0007906	Pa×s	347.28	Joback Method
dvisc	0.0013957	Pa×s	311.35	Joback Method
dvisc	0.0028574	Pa×s	275.43	Joback Method
dvisc	0.0072531	Pa×s	239.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129362&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
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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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