Pivalic acid, 2-methylpropyl ester

Other names:	iso-Butyl pivalate
	Propanoic acid, 2,2-dimethyl, 2-methylpropyl ester
Inchi:	InChI=1S/C9H18O2/c1-7(2)6-11-8(10)9(3,4)5/h7H,6H2,1-5H3
InchiKey:	IFVLZKSUYNTRHJ-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CC(C)COC(=O)C(C)(C)C
Mol. weight [g/mol]:	158.24
CAS:	5129-38-4

Physical Properties

Property code	Value	Unit	Source
gf	-208.62	kJ/mol	Joback Method
hf	-487.92	kJ/mol	Joback Method
hfus	10.92	kJ/mol	Joback Method
hvap	5515.00	kJ/mol	NIST Webbook
log10ws	-1.97		Crippen Method
logp	2.232		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	930.00		NIST Webbook
rinpol	933.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1085.00		NIST Webbook
tb	477.94	K	Joback Method
tc	666.16	K	Joback Method
tf	250.77	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.82	J/mol×K	477.94	Joback Method
cpg	392.85	J/mol×K	634.79	Joback Method

cpg	380.76	J/mol×K	603.42	Joback Method
cpg	368.03	J/mol×K	572.05	Joback Method
cpg	354.64	J/mol×K	540.68	Joback Method
cpg	340.58	J/mol×K	509.31	Joback Method
cpg	404.33	J/mol×K	666.16	Joback Method
dvisc	0.0002253	Pa×s	477.94	Joback Method
dvisc	0.0003117	Pa×s	440.08	Joback Method
dvisc	0.0004585	Pa×s	402.22	Joback Method
dvisc	0.0007309	Pa×s	364.36	Joback Method
dvisc	0.0012980	Pa×s	326.49	Joback Method
dvisc	0.0026801	Pa×s	288.63	Joback Method
dvisc	0.0068881	Pa×s	250.77	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129384&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