Propanoic acid, 1,1-dimethylethyl ester

Other names:	Propionic acid, tert-butyl ester
	tert-Butyl propionate
	C2H5C(O)OC(CH3)3
	t-Butyl propanoate
	t-Butyl propionate
	tert-Butyl propanoate
	1,1-Dimethylethyl propionate
	Propanoic acid, tert-butyl ester
Inchi:	InChI=1S/C7H14O2/c1-5-6(8)9-7(2,3)4/h5H2,1-4H3
InchiKey:	JAELLLITIZHOGQ-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCC(=O)OC(C)(C)C
Mol. weight [g/mol]:	130.18
CAS:	20487-40-5

Physical Properties

Property code	Value	Unit	Source
gf	-223.02	kJ/mol	Joback Method
hf	-441.36	kJ/mol	Joback Method
hfus	9.26	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.738		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	777.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	776.00		NIST Webbook
ripol	964.00		NIST Webbook

ripol	986.00		NIST Webbook
ripol	996.00		NIST Webbook
ripol	998.00		NIST Webbook
ripol	958.00		NIST Webbook
ripol	928.00		NIST Webbook
ripol	964.00		NIST Webbook
ripol	964.00		NIST Webbook
ripol	986.00		NIST Webbook
ripol	967.00		NIST Webbook
ripol	928.00		NIST Webbook
ripol	967.00		NIST Webbook
ripol	967.00		NIST Webbook
ripol	967.00		NIST Webbook
ripol	964.00		NIST Webbook
tb	391.50	K	NIST Webbook
tc	620.42	K	Joback Method
tf	243.23	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.05	J/mol×K	432.62	Joback Method
cpg	253.38	J/mol×K	463.92	Joback Method
cpg	265.15	J/mol×K	495.22	Joback Method
cpg	276.37	J/mol×K	526.52	Joback Method
cpg	287.06	J/mol×K	557.82	Joback Method
cpg	297.22	J/mol×K	589.12	Joback Method
cpg	306.89	J/mol×K	620.42	Joback Method
dvisc	0.0047587	Pa×s	243.23	Joback Method
dvisc	0.0022582	Pa×s	274.80	Joback Method
dvisc	0.0012495	Pa×s	306.36	Joback Method
dvisc	0.0007722	Pa×s	337.93	Joback Method
dvisc	0.0005181	Pa×s	369.49	Joback Method
dvisc	0.0003702	Pa×s	401.06	Joback Method
dvisc	0.0002778	Pa×s	432.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20487405&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume