Propanoic acid, 2,2-dimethyl-, ethyl ester

Other names:	2,2-Dimethylpropanoic acid ethyl ester
	2,2-Dimethylpropionic acid, ethyl ester
	ETHYL 2,2-DIMETHYLPROPIONATE
	ETHYL ESTER PIVALIC ACID
	ETHYL PIVALATE
	Ethyl 2,2-dimethylpropanoate
	Ethyl trimethylacetate
	NSC 17494
	Pivalic acid, ethyl ester
	Trimethylacetic acid, ethyl ester
Inchi:	InChI=1S/C7H14O2/c1-5-9-6(8)7(2,3)4/h5H2,1-4H3
InchiKey:	HHEIMYAXCOIQCJ-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCOC(=O)C(C)(C)C
Mol. weight [g/mol]:	130.18
CAS:	3938-95-2

Physical Properties

Property code	Value	Unit	Source
chl	-4188.50 ± 1.00	kJ/mol	NIST Webbook
chl	-4178.10 ± 8.40	kJ/mol	NIST Webbook
gf	-223.02	kJ/mol	Joback Method
hf	-536.00	kJ/mol	NIST Webbook
hf	-525.60 ± 1.00	kJ/mol	NIST Webbook
hfl	-577.20 ± 8.40	kJ/mol	NIST Webbook
hfl	-566.80 ± 1.00	kJ/mol	NIST Webbook
hfus	9.26	kJ/mol	Joback Method
hvap	41.30 ± 0.10	kJ/mol	NIST Webbook
hvap	4150.00	kJ/mol	NIST Webbook
hvap	41.20	kJ/mol	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	772.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	771.00		NIST Webbook

rinpol	777.00		NIST Webbook
rinpol	776.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	947.00		NIST Webbook
tb	391.50 ± 0.10	K	NIST Webbook
tb	391.55 ± 0.40	K	NIST Webbook
tb	391.20	K	NIST Webbook
tb	391.50	K	KDB
tb	389.65 ± 2.00	K	NIST Webbook
tc	620.42	K	Joback Method
tf	183.60 ± 0.10	K	NIST Webbook
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.89	J/mol×K	620.42	Joback Method
cpg	287.06	J/mol×K	557.82	Joback Method
cpg	297.22	J/mol×K	589.12	Joback Method
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
cpl	251.30	J/mol×K	298.15	NIST Webbook
cpl	277.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0002778	Pa×s	432.62	Joback Method
dvisc	0.0005181	Pa×s	369.49	Joback Method
dvisc	0.0003702	Pa×s	401.06	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
hvapt	33.80 ± 0.60	kJ/mol	368.50	NIST Webbook
hvapt	36.90 ± 0.20	kJ/mol	368.50	NIST Webbook
hvapt	39.80 ± 0.10	kJ/mol	368.50	NIST Webbook

Sources

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1096.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3938952&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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