Propanoic acid, 2-methyl-, propyl ester

Other names:	ISOBUTYRIC ACID N-PROPYL ESTER
	Isobutyric acid, propyl ester
	N-PROPYL 2-METHYLPROPANOATE
	N-Propyl iso-butyrate
	PROPYL ESTER ISOBUTYRIC ACID
	Propyl 2-methylpropanoate
	Propyl isobutanoate
	Propyl isobutyrate
	n-Propyl isobutyrate
Inchi:	InChI=1S/C7H14O2/c1-4-5-9-7(8)6(2)3/h6H,4-5H2,1-3H3
InchiKey:	AZFUASHXSOTBNU-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCCOC(=O)C(C)C
Mol. weight [g/mol]:	130.18
CAS:	644-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2830.00	kPa	KDB
rinpol	862.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	836.00		NIST Webbook

rinpol	841.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	836.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1054.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1051.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1044.00		NIST Webbook
ripol	1044.00		NIST Webbook
ripol	1094.00		NIST Webbook
tb	412.00 ± 2.00	K	NIST Webbook
tb	407.10 ± 0.50	K	NIST Webbook
tb	408.60	K	KDB
tc	581.00	K	KDB
tc	579.40 ± 0.60	K	NIST Webbook
tc	589.20 ± 6.00	K	NIST Webbook
tf	225.81	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/mol×K	435.41	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	301.45	J/mol×K	615.76	Joback Method
dvisc	0.0021099	Pa×s	260.74	Joback Method
dvisc	0.0047724	Pa×s	225.81	Joback Method
dvisc	0.0011312	Pa×s	295.68	Joback Method

dvisc	0.0006919	Pa×s	330.61	Joback Method
dvisc	0.0004649	Pa×s	365.54	Joback Method
dvisc	0.0003348	Pa×s	400.48	Joback Method
dvisc	0.0002542	Pa×s	435.41	Joback Method
hvapt	50.50	kJ/mol	337.00	NIST Webbook
rhol	884.00	kg/m3	273.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.37727e+02
Coeff. B	-1.41868e+04
Coeff. C	-3.38556e+01
Coeff. D	3.12954e-05
Temperature range (K), min.	267.15
Temperature range (K), max.	407.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C644495&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1089
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/mol1089.mol
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
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
pvap:	Vapor pressure
rhol:	Liquid Density
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