Propanoic acid, 2-methylpropyl ester

Other names:	2-METHYLPROPYL PROPIONATE
	2-Methylpropyl propanoate
	ISOBUTYL ESTER PRORIONIC ACID
	ISOBUTYL PROPIONATE
	Isobutyl ester of propanoic acid
	Isobutyl propanoate
	Propionic acid, isobutyl ester
	UN 2394
	iso-Butyl n-propionate
Inchi:	InChI=1S/C7H14O2/c1-4-7(8)9-5-6(2)3/h6H,4-5H2,1-3H3
InchiKey:	FZXRXKLUIMKDEL-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCC(=O)OCC(C)C
Mol. weight [g/mol]:	130.18
CAS:	540-42-1

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
ie	9.94	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2770.00	kPa	KDB
rinpol	848.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	866.00		NIST Webbook

rinpol	853.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	852.80		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	863.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1087.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1091.00		NIST Webbook
tb	409.65 ± 1.00	K	NIST Webbook
tb	410.00	K	NIST Webbook
tb	410.15 ± 1.50	K	NIST Webbook
tb	410.05 ± 1.00	K	NIST Webbook
tb	410.00 ± 0.50	K	NIST Webbook
tb	407.65 ± 1.00	K	NIST Webbook
tb	410.00	K	KDB
tc	592.00	K	KDB
tc	583.80 ± 1.00	K	NIST Webbook
tc	591.90 ± 6.00	K	NIST Webbook
tf	201.70	K	KDB

tf	201.80 ± 0.40	K	NIST Webbook
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
cpg	238.73	J/mol×K	435.41	Joback Method
cpg	301.45	J/mol×K	615.76	Joback Method
dvisc	0.0047724	Pa×s	225.81	Joback Method
dvisc	0.0002542	Pa×s	435.41	Joback Method
dvisc	0.0003348	Pa×s	400.48	Joback Method
dvisc	0.0004649	Pa×s	365.54	Joback Method
dvisc	0.0006919	Pa×s	330.61	Joback Method
dvisc	0.0011312	Pa×s	295.68	Joback Method
dvisc	0.0021099	Pa×s	260.74	Joback Method
hvapt	44.90	kJ/mol	340.50	NIST Webbook
rhol	888.00	kg/m3	273.00	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.70	K	8.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51174e+01
Coeff. B	-3.72389e+03

Coeff. C	-5.53110e+01
Temperature range (K), min.	306.42
Temperature range (K), max.	435.07

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.74201e+01
Coeff. B	-7.80755e+03
Coeff. C	-9.10012e+00
Coeff. D	5.00929e-06
Temperature range (K), min.	271.15
Temperature range (K), max.	583.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1092.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C540421&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1092
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume