Propanoic acid, 2-methyl-, 2-methylpropyl ester

Other names: 2-METHYLPROPYL ISOBUTYRATE
2-Methylpropyl 2-methylpropanoate
2-Methylpropyl 2-methylpropionate
2-methylpropionic acid isobutyl ester
ISOBUTYL ISOBUTANOATE
Isobutyl 2-methylpropanoate
Isobutyl ester of 2-methylpropanoic acid
Isobutyl isobutyrate
Isobutylester kyseliny isomaselne
Isobutyric acid, isobutyl ester
NSC 6538
UN 2528

Inchi: InChI=1S/C8H16O2/c1-6(2)5-10-8(9)7(3)4/h6-7H,5H2,1-4H3

InchiKey: RXGUIWHIADMCFC-UHFFFAOYSA-N

Formula: C8H16O2

SMILES: CC(C)COC(=O)C(C)C

Mol. weight [g/mol]: 144.21

CAS: 97-85-8

Physical Properties

Property code	Value	Unit	Source
chl	-4847.40 ± 1.60	kJ/mol	NIST Webbook
gf	-222.32	kJ/mol	Joback Method
hf	-542.90 ± 1.70	kJ/mol	NIST Webbook
hfl	-587.40 ± 1.60	kJ/mol	NIST Webbook
hfus	12.22	kJ/mol	Joback Method
hvap	44.50 ± 0.10	kJ/mol	NIST Webbook
hvap	44.50	kJ/mol	NIST Webbook
hvap	48.50	kJ/mol	NIST Webbook
hvap	44.49 ± 0.39	kJ/mol	NIST Webbook
log10ws	-1.55		Crippen Method
logp	1.842		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2460.00	kPa	KDB
rinpol	895.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	900.00		NIST Webbook

rinpol	900.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	938.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	913.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	909.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	904.00	NIST Webbook
rinpol	909.00	NIST Webbook
rinpol	914.00	NIST Webbook
rinpol	905.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	913.80	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	906.30	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	902.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	902.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	899.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	900.00	NIST Webbook
rinpol	909.00	NIST Webbook
ripol	1095.00	NIST Webbook
ripol	1092.00	NIST Webbook
ripol	1094.00	NIST Webbook
ripol	1091.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1090.00	NIST Webbook
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ripol	1089.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1103.50		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1081.00		NIST Webbook
ripol	1090.00		NIST Webbook
tb	420.70	K	NIST Webbook
tb	421.80	K	KDB
tb	422.20 ± 2.00	K	NIST Webbook
tb	420.65 ± 1.50	K	NIST Webbook
tb	421.80 ± 0.25	K	NIST Webbook
tb	420.50 ± 0.50	K	NIST Webbook
tb	420.50 ± 0.50	K	NIST Webbook
tb	420.15 ± 1.50	K	NIST Webbook
tc	602.00	K	KDB
tc	601.89 ± 6.00	K	NIST Webbook
tf	192.40	K	KDB
tf	192.50 ± 0.15	K	NIST Webbook
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.42	J/mol×K	640.65	Joback Method
cpg	292.89	J/mol×K	488.32	Joback Method
cpg	305.35	J/mol×K	518.78	Joback Method
cpg	317.32	J/mol×K	549.25	Joback Method
cpg	328.83	J/mol×K	579.72	Joback Method
cpg	339.86	J/mol×K	610.19	Joback Method
cpg	279.95	J/mol×K	457.85	Joback Method
dvisc	0.0003141	Pa×s	418.56	Joback Method
dvisc	0.0004562	Pa×s	379.26	Joback Method
dvisc	0.0007223	Pa×s	339.97	Joback Method

dvisc	0.0012896	Pa×s	300.67	Joback Method
dvisc	0.0027406	Pa×s	261.38	Joback Method
dvisc	0.0002306	Pa×s	457.85	Joback Method
dvisc	0.0076048	Pa×s	222.08	Joback Method
hvapt	46.90	kJ/mol	349.00	NIST Webbook
pvap	0.60	kPa	298.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.14	kPa	308.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.36	kPa	311.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.50	kPa	313.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.85	kPa	316.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	2.22	kPa	319.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.43	kPa	293.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.30	kPa	288.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.21	kPa	283.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
pvap	0.15	kPa	278.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
pvap	0.13	kPa	276.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
pvap	0.11	kPa	274.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
pvap	0.83	kPa	303.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters	
rhol	875.00	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	7.73503e+01
Coeff. B	-8.03882e+03
Coeff. C	-9.01363e+00
Coeff. D	4.18948e-06
Temperature range (K), min.	192.45
Temperature range (K), max.	602.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97858&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters:	https://www.doi.org/10.1016/j.fluid.2008.02.001
Liquid-liquid equilibrium for the system of ionic liquid [BMIm][HSO4] catalysed isobutyl isobutyrate formation:	https://www.doi.org/10.1016/j.jct.2018.03.015
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1104
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1104.mol

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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