Propanoic acid, 2-methyl-, butyl ester

Other names:	Butyl 2-methylpropanoate
	Butyl ester of 2-methylpropanoic acid
	Butyl isobutanoate
	Butyl isobutyrate
	Isobutyric acid n-butyl ester
	Isobutyric acid, butyl ester
	n-Butyl isobutyrate
Inchi:	InChI=1S/C8H16O2/c1-4-5-6-10-8(9)7(2)3/h7H,4-6H2,1-3H3
InchiKey:	JSLCOZYBKYHZNL-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCOC(=O)C(C)C
Mol. weight [g/mol]:	144.21
CAS:	97-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-219.88	kJ/mol	Joback Method
hf	-458.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	936.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	935.00		NIST Webbook

rinpol	895.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	937.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1154.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1129.00		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1145.00		NIST Webbook
tb	458.29	K	Joback Method
tc	637.16	K	Joback Method
tf	237.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method

cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	338.23	J/mol×K	607.34	Joback Method
cpg	348.57	J/mol×K	637.16	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43827e+01
Coeff. B	-3.66957e+03
Coeff. C	-6.01760e+01
Temperature range (K), min.	320.52
Temperature range (K), max.	464.71

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97870&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor 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