Butanoic acid, 2-methylpropyl ester

Other names:	2-METHYLPROPYL BUTYRATE
	2-Methylpropyl butanoate
	Butanoic acid, methyl propyl ester
	Butyric acid, isobutyl ester
	ISOBUTYL BUTYRATE
	ISOBUTYL N-BUTYRATE
	Isobutyl butanoate
	Isobutyl ester of butanoic acid
	NSC 406938
	n-Butyric acid isobutyl ester
Inchi:	InChI=1S/C8H16O2/c1-4-5-8(9)10-6-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	RGFNRWTWDWVHDD-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCC(=O)OCC(C)C
Mol. weight [g/mol]:	144.21
CAS:	539-90-2

Physical Properties

Property code	Value	Unit	Source
chl	-4837.10	kJ/mol	NIST Webbook
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	2450.00	kPa	KDB
rinpol	933.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	937.00		NIST Webbook

rinpol	937.00	NIST Webbook
rinpol	945.00	NIST Webbook
rinpol	945.00	NIST Webbook
rinpol	945.00	NIST Webbook
rinpol	946.00	NIST Webbook
rinpol	935.00	NIST Webbook
rinpol	933.00	NIST Webbook
rinpol	920.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	939.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	961.00	NIST Webbook
rinpol	953.00	NIST Webbook
rinpol	946.00	NIST Webbook
rinpol	946.00	NIST Webbook
rinpol	961.00	NIST Webbook
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rinpol	933.00	NIST Webbook
rinpol	941.00	NIST Webbook
rinpol	940.00	NIST Webbook
rinpol	939.00	NIST Webbook
rinpol	956.00	NIST Webbook
rinpol	933.00	NIST Webbook
rinpol	946.00	NIST Webbook
rinpol	930.00	NIST Webbook
rinpol	940.30	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	920.00	NIST Webbook
rinpol	939.00	NIST Webbook
ripol	1165.00	NIST Webbook
ripol	1139.00	NIST Webbook
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ripol	1146.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1162.00		NIST Webbook
tb	430.10	K	KDB
tc	611.40 ± 6.00	K	NIST Webbook
tc	611.00	K	KDB
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	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0048246	Pa×s	237.08	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
hvapt	41.70	kJ/mol	353.50	NIST Webbook
rhol	863.00	kg/m3	291.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49752e+01
Coeff. B	-3.82371e+03
Coeff. C	-6.07040e+01
Temperature range (K), min.	321.04
Temperature range (K), max.	456.38

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-2.82579e+01
Coeff. B	-3.31903e+03
Coeff. C	6.90926e+00
Coeff. D	-7.79519e-06
Temperature range (K), min.	277.15
Temperature range (K), max.	603.00

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/research/kdb/hcprop/showprop.php?cmpid=1103

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C539902&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=1103

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
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