

Butanoic acid, 2-methyl-, ethyl ester

Other names:	2-Methylbutanoic acid ethyl ester Butyric acid, 2-methyl-, ethyl ester Ethyl «alpha»-methylbutyrate NSC 1103 ethyl 2-methylbutanoate ethyl 2-methylbutyrate
Inchi:	InChI=1S/C7H14O2/c1-4-6(3)7(8)9-5-2/h6H,4-5H2,1-3H3
InchiKey:	HCRBXQFHJMCTLF-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCOC(=O)C(C)CC
Mol. weight [g/mol]:	130.18
CAS:	7452-79-1

Physical Properties

Property code	Value	Unit	Source
chl	-4188.60 ± 8.40	kJ/mol	NIST Webbook
chl	-4195.00 ± 1.30	kJ/mol	NIST Webbook
gf	-228.30	kJ/mol	Joback Method
hf	-522.60 ± 8.80	kJ/mol	NIST Webbook
hf	-516.10 ± 1.40	kJ/mol	NIST Webbook
hfl	-560.40 ± 1.40	kJ/mol	NIST Webbook
hfus	13.15	kJ/mol	Joback Method
hvap	44.30 ± 0.30	kJ/mol	NIST Webbook
hvap	44.00 ± 1.00	kJ/mol	NIST Webbook
hvap	64.70	kJ/mol	NIST Webbook
hvap	44.30	kJ/mol	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	850.00		NIST Webbook
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tb	405.60	K	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tb	406.20	K	NIST Webbook
tb	406.05 ± 0.40	K	NIST Webbook
tc	615.76	K	Joback Method
tf	225.81	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.45	J/mol×K	615.76	Joback Method
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
cpl	327.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0005320	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005030	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004760	Pa×s	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0005630	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008310	Pa×s	293.15	Density and Viscosity of Binary Mixtures of Ethyl-2-methylbutyrate and Ethyl Hexanoate with Methanol, Ethanol, and 1-Propanol at (293.15, 303.15, and 313.15) K
dvisc	0.0007230	Pa×s	303.15	Density and Viscosity of Binary Mixtures of Ethyl-2-methylbutyrate and Ethyl Hexanoate with Methanol, Ethanol, and 1-Propanol at (293.15, 303.15, and 313.15) K

dvisc	0.0006350	Pa×s	313.15	Density and Viscosity of Binary Mixtures of Ethyl-2-methylbutyrate and Ethyl Hexanoate with Methanol, Ethanol, and 1-Propanol at (293.15, 303.15, and 313.15) K
dvisc	0.0005970	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006350	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006770	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007230	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007740	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008310	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0004520	Pa×s	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	362.10	K	24.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	371.20	K	34.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	378.30	K	43.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	384.20	K	53.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	389.50	K	62.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	394.00	K	72.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	397.90	K	81.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa

tdp	401.80	K	91.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tdp	408.70	K	110.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tdp	411.70	K	119.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tdp	414.50	K	129.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tdp	417.30	K	138.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tdp	420.10	K	148.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tdp	422.50	K	157.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa

tbp	424.80	K	167.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	427.00	K	176.50	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	429.10	K	186.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa
tbp	429.90	K	190.00	Vapor pressure data for ethyl-2-methylbutyrate, hexanal and (E)-2-hexenal at a pressure range of (25 to 190) kPa

Sources

Crippen Method:
Joback Method:
High-pressure (vapor + liquid) equilibria for binary systems containing a viscosity of binary mixtures of ethyl-2-methylbutyrate and ethyl-2-methylbutyrate, hexanal, and (E)-2-hexenal at pressures of 25, 50, 75, and 100 kPa; Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters;
Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws
https://en.wikipedia.org/wiki/Joback_method
<https://www.doi.org/10.1016/j.jct.2017.08.008>
<https://www.doi.org/10.1021/je0500633>
<https://www.doi.org/10.1016/j.jct.2014.03.006>
<http://link.springer.com/article/10.1007/BF02311772>
<https://www.doi.org/10.1021/je050001c>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C7452791&Units=SI>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

chl:

Standard liquid enthalpy of combustion

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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