Butanoic acid, 3-methyl-, methyl ester

Other names:	3-Methylbutanoic acid methyl ester
	Isovaleric acid, methyl ester
	Methyl 3-methylbutanoate
	Methyl 3-methylbutyrate
	Methyl isopentanoate
	UN 2400
Inchi:	InChI=1S/C6H12O2/c1-5(2)4-6(7)8-3/h5H,4H2,1-3H3
InchiKey:	OQAGVSWESNCJJT-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	COC(=O)CC(C)C
Mol. weight [g/mol]:	116.16
CAS:	556-24-1

Physical Properties

Property code	Value	Unit	Source
af	0.4054		Cheméo Relay (1.0)
chl	-3537.20 ± 7.10	kJ/mol	NIST Webbook
hf	-497.90 ± 7.50	kJ/mol	NIST Webbook
hfl	-538.90 ± 7.10	kJ/mol	NIST Webbook
hfus	10.56	kJ/mol	Joback Method
hvap	41.00	kJ/mol	NIST Webbook
hvap	41.00 ± 1.00	kJ/mol	NIST Webbook
ie	9.91	eV	Cheméo Relay (1.0)
log10ws	-1.30		Cheméo Relay (1.0)
logp	1.206		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	775.10		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	775.10		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	781.30		NIST Webbook
rinpol	775.00		NIST Webbook

rinpol	785.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	741.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	754.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	793.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	761.00	NIST Webbook
rinpol	761.30	NIST Webbook
rinpol	761.30	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	765.00	NIST Webbook
ripol	1021.00	NIST Webbook
ripol	1016.00	NIST Webbook
ripol	1022.00	NIST Webbook
ripol	1019.00	NIST Webbook
ripol	1025.00	NIST Webbook
ripol	1022.00	NIST Webbook
ripol	1019.00	NIST Webbook
ripol	1059.00	NIST Webbook
ripol	1013.00	NIST Webbook
ripol	1011.00	NIST Webbook

ripol	1017.00		NIST Webbook
ripol	1010.00		NIST Webbook
ripol	1020.00		NIST Webbook
ripol	1010.00		NIST Webbook
ripol	1019.00		NIST Webbook
ripol	1019.00		NIST Webbook
ripol	1018.00		NIST Webbook
ripol	1013.00		NIST Webbook
ripol	1019.00		NIST Webbook
ripol	1020.00		NIST Webbook
ripol	1015.00		NIST Webbook
ripol	1016.00		NIST Webbook
ripol	1017.00		NIST Webbook
ripol	1012.00		NIST Webbook
ripol	1014.00		NIST Webbook
ripol	1020.00		NIST Webbook
ripol	1014.00		NIST Webbook
ripol	1008.00		NIST Webbook
ripol	1025.00		NIST Webbook
tb	389.00 ± 2.00	K	NIST Webbook
tb	389.65 ± 0.50	K	NIST Webbook
tb	389.50 ± 0.50	K	NIST Webbook
tb	388.70 ± 1.50	K	NIST Webbook
tb	390.55 ± 0.40	K	NIST Webbook
tb	389.70	K	NIST Webbook
tc	561.63	K	Cheméo Relay (1.0)
tf	182.42	K	Cheméo Relay (1.0)
vc	0.375	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.38	J/mol×K	563.94	Joback Method
cpg	255.87	J/mol×K	594.22	Joback Method
cpg	210.06	J/mol×K	442.81	Joback Method
cpg	219.89	J/mol×K	473.09	Joback Method
cpg	229.39	J/mol×K	503.38	Joback Method
cpg	238.55	J/mol×K	533.66	Joback Method
cpg	199.90	J/mol×K	412.53	Joback Method
dvisc	0.0011317	Pa×s	280.54	Joback Method
dvisc	0.0020807	Pa×s	247.54	Joback Method

dvisc	0.0046134	Pa×s	214.54	Joback Method
dvisc	0.0006998	Pa×s	313.53	Joback Method
dvisc	0.0004742	Pa×s	346.53	Joback Method
dvisc	0.0003438	Pa×s	379.53	Joback Method
dvisc	0.0002624	Pa×s	412.53	Joback Method
hvapt	41.20	kJ/mol	322.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47972e+01
Coeff. B	-3.46759e+03
Coeff. C	-4.93340e+01
Temperature range (K), min.	288.32
Temperature range (K), max.	414.89

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C556241&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity

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
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
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