Methyl isobutyrate

Other names:	(CH3)2CHC(O)OCH3
	Isobutyric acid, methyl ester
	METHYL 2-METHYLPROPANOATE
	METHYL ESTER ISOBUTYRIC ACID
	METHYL ISOBUTANOATE
	Methyl 2-methylpropionate
	Methyl methylpropanoate
	Methylester kyseliny isomaselne
	NSC 126780
	Propanoic acid, 2-methyl-, methyl ester
Inchi:	InChI=1S/C5H10O2/c1-4(2)5(6)7-3/h4H,1-3H3
InchiKey:	BHIWKHZACMWKOJ-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	COC(=O)C(C)C
Mol. weight [g/mol]:	102.13
CAS:	547-63-7

Physical Properties

Property code	Value	Unit	Source
af	0.3620		KDB
affp	836.60	kJ/mol	NIST Webbook
basg	805.70	kJ/mol	NIST Webbook
dm	2.00	debye	KDB
gf	-245.14	kJ/mol	Joback Method
hf	-396.61	kJ/mol	Joback Method
hfus	7.97	kJ/mol	Joback Method
hvap	37.42	kJ/mol	NIST Webbook
hvap	33.40 ± 0.02	kJ/mol	NIST Webbook
ie	9.86	eV	NIST Webbook
ie	9.98 ± 0.02	eV	NIST Webbook
log10ws	-0.54		Crippen Method
logp	0.815		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3430.40 ± 40.00	kPa	NIST Webbook
pc	3432.00 ± 81.06	kPa	NIST Webbook
pc	3430.00	kPa	KDB
rhoc	301.70 ± 4.09	kg/m3	NIST Webbook

rhoc	301.19 ± 10.01	kg/m3	NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	670.00		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	681.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	691.60		NIST Webbook
rinpol	673.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	690.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	903.00		NIST Webbook
ripol	913.00		NIST Webbook
ripol	940.00		NIST Webbook
ripol	922.00		NIST Webbook
ripol	920.00		NIST Webbook
ripol	913.00		NIST Webbook
ripol	924.00		NIST Webbook

ripol	924.00		NIST Webbook
ripol	919.00		NIST Webbook
ripol	922.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	921.00		NIST Webbook
ripol	927.00		NIST Webbook
ripol	919.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	903.00		NIST Webbook
ripol	924.00		NIST Webbook
ripol	924.00		NIST Webbook
ripol	916.00		NIST Webbook
ripol	910.00		NIST Webbook
ripol	924.00		NIST Webbook
ripol	900.00		NIST Webbook
ripol	915.00		NIST Webbook
tb	365.50	K	NIST Webbook
tb	363.20	K	NIST Webbook
tb	372.15 ± 1.00	K	NIST Webbook
tb	365.15 ± 2.00	K	NIST Webbook
tb	367.00 ± 2.00	K	NIST Webbook
tb	355.70 ± 0.50	K	NIST Webbook
tb	365.45 ± 1.00	K	NIST Webbook
tb	365.50 ± 0.50	K	NIST Webbook
tb	365.45 ± 1.00	K	NIST Webbook
tb	365.70 ± 0.30	K	NIST Webbook
tb	364.95 ± 2.00	K	NIST Webbook
tb	384.55 ± 1.00	K	NIST Webbook
tb	365.45 ± 1.00	K	NIST Webbook
tb	365.60	K	KDB
tb	365.00 ± 1.00	K	NIST Webbook
tb	365.45 ± 1.00	K	NIST Webbook
tb	365.60	K	NIST Webbook
tb	365.55 ± 1.00	K	NIST Webbook
tc	540.80	K	KDB
tc	546.80 ± 6.00	K	NIST Webbook
tc	540.70 ± 1.00	K	NIST Webbook
tc	540.70 ± 1.00	K	NIST Webbook
tf	187.15 ± 1.50	K	NIST Webbook
tf	188.50 ± 0.25	K	NIST Webbook
tf	188.40	K	KDB
vc	0.339	m3/kmol	KDB
zc	0.2585950		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.90	J/mol×K	481.06	Joback Method
cpg	211.93	J/mol×K	572.47	Joback Method
cpg	204.52	J/mol×K	542.00	Joback Method
cpg	196.85	J/mol×K	511.53	Joback Method
cpg	163.44	J/mol×K	389.65	Joback Method
cpg	172.19	J/mol×K	420.12	Joback Method
cpg	180.68	J/mol×K	450.59	Joback Method
dvisc	0.0002653	Pa×s	389.65	Joback Method
dvisc	0.0006915	Pa×s	296.46	Joback Method
dvisc	0.0004730	Pa×s	327.52	Joback Method
dvisc	0.0003455	Pa×s	358.59	Joback Method
dvisc	0.0043372	Pa×s	203.27	Joback Method
dvisc	0.0019995	Pa×s	234.33	Joback Method
dvisc	0.0011050	Pa×s	265.40	Joback Method
hvapt	40.10	kJ/mol	302.50	NIST Webbook
hvapt	33.70	kJ/mol	449.50	NIST Webbook
hvapt	32.61	kJ/mol	365.60	NIST Webbook
rhol	891.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48798e+01
Coeff. B	-3.30681e+03
Coeff. C	-4.27450e+01
Temperature range (K), min.	269.36
Temperature range (K), max.	388.34

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.51167e+01

Coeff. B	-7.28577e+03
Coeff. C	-1.04269e+01
Coeff. D	7.17430e-06
Temperature range (K), min.	239.15
Temperature range (K), max.	535.58

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1064
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C547637&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=1064
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
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
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
rhoc:	Critical density
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
zc:	Critical Compressibility