

Butanoic acid, 2-methyl-, methyl ester

Other names:	Butyric acid, 2-methyl-, methyl ester Methyl «alpha»-methylbutanoate Methyl «alpha»-methylbutyrate Methyl 2-methylbutanoate Methyl 2-methylbutyrate 2-Methylbutanoic acid, methyl ester dl-2-Methylbutyric acid methyl ester Methyl ester of 2-methyl-butanoic acid 2-Methylbutyric acid, methyl ester Butyric acid, «alpha»-methyl-, methyl ester 2-methyl(methyl butanoate)
Inchi:	InChI=1S/C6H12O2/c1-4-5(2)6(7)8-3/h5H,4H2,1-3H3
InchiKey:	OCWLYWIFNDCWRZ-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCC(C)C(=O)OC
Mol. weight [g/mol]:	116.16
CAS:	868-57-5

Physical Properties

Property code	Value	Unit	Source
chl	-3541.80 ± 7.10	kJ/mol	NIST Webbook
gf	-236.72	kJ/mol	Joback Method
hf	-492.50 ± 7.50	kJ/mol	NIST Webbook
hfl	-534.30 ± 7.10	kJ/mol	NIST Webbook
hfus	10.56	kJ/mol	Joback Method
hvap	42.00 ± 1.00	kJ/mol	NIST Webbook
hvap	41.80	kJ/mol	NIST Webbook
log10ws	-0.95		Crippen Method
logp	1.205		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpola	771.00		NIST Webbook
rinpola	754.00		NIST Webbook
rinpola	779.00		NIST Webbook
rinpola	754.00		NIST Webbook
rinpola	777.00		NIST Webbook
rinpola	760.00		NIST Webbook

rinpol	778.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	783.10	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	786.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	764.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	781.70	NIST Webbook
rinpol	785.00	NIST Webbook
rinpol	770.00	NIST Webbook
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ripol	1008.00	NIST Webbook
ripol	1014.00	NIST Webbook
ripol	1049.00	NIST Webbook
ripol	1052.00	NIST Webbook
ripol	1002.00	NIST Webbook
ripol	1009.00	NIST Webbook
ripol	1000.00	NIST Webbook
ripol	1004.00	NIST Webbook
ripol	1010.00	NIST Webbook
ripol	983.00	NIST Webbook
ripol	989.00	NIST Webbook
ripol	1007.00	NIST Webbook
ripol	1009.00	NIST Webbook

ripol	1007.00	NIST Webbook
ripol	980.00	NIST Webbook
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ripol	1008.00	NIST Webbook
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ripol	1004.00	NIST Webbook
ripol	1016.00	NIST Webbook
ripol	978.00	NIST Webbook
ripol	999.00	NIST Webbook
ripol	1005.00	NIST Webbook
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ripol	1003.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	1022.00		NIST Webbook
ripol	1007.00		NIST Webbook
tb	389.05 ± 0.40	K	NIST Webbook
tb	388.00 ± 1.50	K	NIST Webbook
tc	594.22	K	Joback Method
tf	214.54	K	Joback Method
vc	0.390	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.90	J/mol×K	412.53	Joback Method
cpg	247.38	J/mol×K	563.94	Joback Method
cpg	238.55	J/mol×K	533.66	Joback Method
cpg	229.39	J/mol×K	503.38	Joback Method
cpg	219.89	J/mol×K	473.09	Joback Method
cpg	210.06	J/mol×K	442.81	Joback Method
cpg	255.87	J/mol×K	594.22	Joback Method
dvisc	0.0002624	Paxs	412.53	Joback Method
dvisc	0.0003438	Paxs	379.53	Joback Method
dvisc	0.0004742	Paxs	346.53	Joback Method
dvisc	0.0006998	Paxs	313.53	Joback Method
dvisc	0.0011317	Paxs	280.54	Joback Method
dvisc	0.0020807	Paxs	247.54	Joback Method
dvisc	0.0046134	Paxs	214.54	Joback Method

Sources

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C868575&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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