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)
	Butanoic acid, 2-methyl-, methyl ester, (.+/-.)-
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:	53955-81-0

Physical Properties

Property code	Value	Unit	Source
gf	-236.72	kJ/mol	Joback Method
hf	-417.25	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	37.72	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	1.205		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	388.20	K	NIST Webbook
tc	594.22	K	Joback Method
tf	214.54	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.90	J/mol×K	412.53	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	247.38	J/mol×K	563.94	Joback Method
cpg	255.87	J/mol×K	594.22	Joback Method
dvisc	0.0046134	Pa×s	214.54	Joback Method
dvisc	0.0020807	Pa×s	247.54	Joback Method
dvisc	0.0011317	Pa×s	280.54	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

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53955810&Units=SI

Legend

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume