Butanoic acid, 2-hydroxy-3-methyl-, methyl ester

Other names: Butanoic acid, 2-hydroxy-3-methyl-, methyl ester
Methyl 2-hydroxy-3-methylbutanoate
Methyl 2-hydroxy-3-methylbutyrate
Methyl 3-methyl 2-hydroxybutanoate

Inchi: InChI=1S/C6H12O3/c1-4(2)5(7)6(8)9-3/h4-5,7H,1-3H3

InchiKey: YSGBMDFJWFIEDF-UHFFFAOYSA-N

Formula: C6H12O3

SMILES: COC(=O)C(O)C(C)C

Mol. weight [g/mol]: 132.16

Physical Properties

Property code	Value	Unit	Source
af	0.5976		Cheméo Relay (1.0)
hf	-659.65	kJ/mol	Cheméo Relay (1.0)
hfus	11.12	kJ/mol	Joback Method
hvap	60.09	kJ/mol	Cheméo Relay (1.0)
ie	10.16	eV	Cheméo Relay (1.0)
logp	0.176		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	889.00		NIST Webbook
rinpol	889.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1383.00		NIST Webbook
tb	420.72	K	Cheméo Relay (1.0)
tc	623.23	K	Cheméo Relay (1.0)
tf	290.08	K	Cheméo Relay (1.0)
vc	0.396	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.04	J/mol×K	504.27	Joback Method
cpg	255.38	J/mol×K	533.92	Joback Method
cpg	264.36	J/mol×K	563.56	Joback Method
cpg	272.99	J/mol×K	593.21	Joback Method
cpg	281.27	J/mol×K	622.85	Joback Method
cpg	289.19	J/mol×K	652.50	Joback Method
cpg	296.77	J/mol×K	682.14	Joback Method
dvisc	0.0398736	Pa×s	260.36	Joback Method
dvisc	0.0082434	Pa×s	301.01	Joback Method
dvisc	0.0024799	Pa×s	341.66	Joback Method
dvisc	0.0009632	Pa×s	382.31	Joback Method
dvisc	0.0004487	Pa×s	422.97	Joback Method
dvisc	0.0002390	Pa×s	463.62	Joback Method
dvisc	0.0001409	Pa×s	504.27	Joback Method

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17417004&Units=SI

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
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