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

Other names: methyl 2-hydroxy-2-methylbutanoate
Inchi: InChI=1S/C6H12O3/c1-4-6(2,8)5(7)9-3/h8H,4H2,1-3H3
InchiKey: FMXYCZVOMYLMKM-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: CCC(C)(O)C(=O)OC
Mol. weight [g/mol]: 132.16
CAS: 32793-34-3

Physical Properties

Property code	Value	Unit	Source
gf	-368.26	kJ/mol	Joback Method
hf	-572.95	kJ/mol	Joback Method
hfus	10.76	kJ/mol	Joback Method
hvap	53.49	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	923.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1272.00		NIST Webbook
tb	501.92	K	Joback Method
tc	682.72	K	Joback Method
tf	292.78	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.95	J/mol×K	501.92	Joback Method
cpg	292.32	J/mol×K	652.58	Joback Method
cpg	284.51	J/mol×K	622.45	Joback Method
cpg	276.27	J/mol×K	592.32	Joback Method
cpg	267.61	J/mol×K	562.19	Joback Method

cpg	258.51	J/mol×K	532.05	Joback Method
cpg	299.73	J/mol×K	682.72	Joback Method
dvisc	0.0001543	Pa×s	501.92	Joback Method
dvisc	0.0002484	Pa×s	467.06	Joback Method
dvisc	0.0004319	Pa×s	432.21	Joback Method
dvisc	0.0008275	Pa×s	397.35	Joback Method
dvisc	0.0017968	Pa×s	362.49	Joback Method
dvisc	0.0046012	Pa×s	327.64	Joback Method
dvisc	0.0147388	Pa×s	292.78	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32793343&Units=SI
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

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
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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