methyl 3-hydroxy-2-methylbutanoate

Other names: methyl 3-hydroxy-2-methylbutyrate
Inchi: InChI=1S/C6H12O3/c1-4(5(2)7)6(8)9-3/h4-5,7H,1-3H3
InchiKey: FFJMPYODEQVBEX-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: COC(=O)C(C)C(C)O
Mol. weight [g/mol]: 132.16

Physical Properties

Property code	Value	Unit	Source
gf	-375.98	kJ/mol	Joback Method
hf	-574.76	kJ/mol	Joback Method
hfus	11.12	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.176		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	930.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	901.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1519.00		NIST Webbook
tb	504.27	K	Joback Method
tc	682.14	K	Joback Method
tf	260.36	K	Joback Method
vc	0.403	m3/kmol	Joback Method

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

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=R319474&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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