Pentanoic acid, 2-hydroxy-4-methyl-, methyl ester

Other names: Valeric acid, 2-hydroxy-4-methyl-, methyl ester
methyl 2-hydroxy-4-methylpentanoate
2-Hydroxyisocaproic acid, methyl ester
methyl 2-hydroxy-4-methylvalerate

Inchi: InChI=1S/C7H14O3/c1-5(2)4-6(8)7(9)10-3/h5-6,8H,4H2,1-3H3

InchiKey: JOSNYUDSMPILKL-UHFFFAOYSA-N

Formula: C7H14O3

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

Mol. weight [g/mol]: 146.18

CAS: 40348-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-367.56	kJ/mol	Joback Method
hf	-595.40	kJ/mol	Joback Method
hfus	13.71	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.566		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1013.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	994.90		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1516.00		NIST Webbook
tb	527.15	K	Joback Method
tc	703.42	K	Joback Method
tf	271.63	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.08	J/mol×K	527.15	Joback Method
cpg	299.43	J/mol×K	556.53	Joback Method
cpg	309.37	J/mol×K	585.91	Joback Method
cpg	318.91	J/mol×K	615.28	Joback Method
cpg	328.05	J/mol×K	644.66	Joback Method
cpg	336.78	J/mol×K	674.04	Joback Method
cpg	345.13	J/mol×K	703.42	Joback Method
dvisc	0.0314993	Pa×s	271.63	Joback Method
dvisc	0.0065975	Pa×s	314.22	Joback Method
dvisc	0.0020069	Pa×s	356.80	Joback Method
dvisc	0.0007868	Pa×s	399.39	Joback Method
dvisc	0.0003695	Pa×s	441.98	Joback Method
dvisc	0.0001982	Pa×s	484.56	Joback Method
dvisc	0.0001175	Pa×s	527.15	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=C40348729&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
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