4-Methyl-2-oxovaleric acid

Other names:	Isopropylpyruvic acid
	2-Keto-4-methylpentanoic acid
	Pentanoic acid, 4-methyl-2-oxo-
	«alpha»-Ketoisocaproic acid
	4-methyl-2-oxopentanoic acid
Inchi:	InChI=1S/C6H10O3/c1-4(2)3-5(7)6(8)9/h4H,3H2,1-2H3,(H,8,9)
InchiKey:	BKAJNAXTPSGJCU-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CC(C)CC(=O)C(=O)O
Mol. weight [g/mol]:	130.14
CAS:	816-66-0

Physical Properties

Property code	Value	Unit	Source
gf	-397.46	kJ/mol	Joback Method
hf	-549.84	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	58.73	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	0.686		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	536.16	K	Joback Method
tc	720.16	K	Joback Method
tf	303.06	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.83	J/mol×K	536.16	Joback Method
cpg	275.12	J/mol×K	689.50	Joback Method
cpg	268.22	J/mol×K	658.83	Joback Method
cpg	260.95	J/mol×K	628.16	Joback Method

cpg	253.30	J/mol×K	597.49	Joback Method
cpg	245.27	J/mol×K	566.83	Joback Method
cpg	281.66	J/mol×K	720.16	Joback Method
dvisc	0.0001647	Pa×s	536.16	Joback Method
dvisc	0.0002596	Pa×s	497.31	Joback Method
dvisc	0.0004422	Pa×s	458.46	Joback Method
dvisc	0.0008313	Pa×s	419.61	Joback Method
dvisc	0.0017774	Pa×s	380.76	Joback Method
dvisc	0.0045167	Pa×s	341.91	Joback Method
dvisc	0.0145779	Pa×s	303.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C816660&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume