2-Oxo-4-methylvaleric 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

Physical Properties

Property code	Value	Unit	Source
af	0.6818		Cheméo Relay (1.0)
hf	-602.20	kJ/mol	Cheméo Relay (1.0)
hfus	15.06	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
log10ws	-0.67		Cheméo Relay (1.0)
logp	0.686		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	464.56	K	Cheméo Relay (1.0)
tc	660.76	K	Cheméo Relay (1.0)
tf	305.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.83	J/mol×K	536.16	Joback Method
cpg	245.27	J/mol×K	566.83	Joback Method
cpg	253.30	J/mol×K	597.49	Joback Method
cpg	260.95	J/mol×K	628.16	Joback Method
cpg	268.22	J/mol×K	658.83	Joback Method

cpg	275.12	J/mol×K	689.50	Joback Method
cpg	281.66	J/mol×K	720.16	Joback Method
dvisc	0.0145779	Pa×s	303.06	Joback Method
dvisc	0.0045167	Pa×s	341.91	Joback Method
dvisc	0.0017774	Pa×s	380.76	Joback Method
dvisc	0.0008313	Pa×s	419.61	Joback Method
dvisc	0.0004422	Pa×s	458.46	Joback Method
dvisc	0.0002596	Pa×s	497.31	Joback Method
dvisc	0.0001647	Pa×s	536.16	Joback Method

Sources

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=C816660&Units=SI
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

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
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

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