2,3-Pentanedione, 4-methyl-

Other names:	Acetyl isobutyryl
	4-Methyl-2,3-pentanedione
	4-Methylpentane-2,3-dione
	Isopropyl methyl diketone
	Methyl isopropyl diketone
Inchi:	InChI=1S/C6H10O2/c1-4(2)6(8)5(3)7/h4H,1-3H3
InchiKey:	JENYBWHRLYZSSZ-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CC(=O)C(=O)C(C)C
Mol. weight [g/mol]:	114.14
CAS:	7493-58-5

Physical Properties

Property code	Value	Unit	Source
gf	-260.64	kJ/mol	Joback Method
hf	-397.61	kJ/mol	Joback Method
hfus	10.97	kJ/mol	Joback Method
hvap	42.05	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.801		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	763.00		NIST Webbook
rinpol	763.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1046.00		NIST Webbook
tb	443.98	K	Joback Method
tc	638.05	K	Joback Method
tf	242.24	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	193.74	J/mol×K	443.98	Joback Method
cpg	203.55	J/mol×K	476.32	Joback Method
cpg	212.92	J/mol×K	508.67	Joback Method
cpg	221.86	J/mol×K	541.01	Joback Method
cpg	230.38	J/mol×K	573.36	Joback Method
cpg	238.49	J/mol×K	605.70	Joback Method
cpg	246.20	J/mol×K	638.05	Joback Method
dvisc	0.0048342	Pa×s	242.24	Joback Method
dvisc	0.0023833	Pa×s	275.86	Joback Method
dvisc	0.0013702	Pa×s	309.49	Joback Method
dvisc	0.0008780	Pa×s	343.11	Joback Method
dvisc	0.0006091	Pa×s	376.73	Joback Method
dvisc	0.0004487	Pa×s	410.36	Joback Method
dvisc	0.0003462	Pa×s	443.98	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=C7493585&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