2,4-Pentanedione, 3-acetyl-

Other names:	3-Acetyl-2,4-pentanedione
	Methane, triacetyl-
	Triacetylmethane
	Methane triacetate
	methine triacetate
Inchi:	InChI=1S/C7H10O3/c1-4(8)7(5(2)9)6(3)10/h7H,1-3H3
InchiKey:	AUZFRUHVDNDVJI-UHFFFAOYSA-N
Formula:	C7H10O3
SMILES:	CC(=O)C(C(C)=O)C(C)=O
Mol. weight [g/mol]:	142.15
CAS:	815-68-9

Physical Properties

Property code	Value	Unit	Source
gf	-381.14	kJ/mol	Joback Method
hf	-530.83	kJ/mol	Joback Method
hfus	15.16	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	0.370		Crippen Method
mcvol	114.200	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	476.70	K	NIST Webbook
tc	722.40	K	Joback Method
tf	303.44	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.37	J/mol×K	520.73	Joback Method
cpg	258.53	J/mol×K	554.34	Joback Method
cpg	268.18	J/mol×K	587.95	Joback Method
cpg	277.31	J/mol×K	621.57	Joback Method

cpg	285.95	J/mol×K	655.18	Joback Method
cpg	294.09	J/mol×K	688.79	Joback Method
cpg	301.76	J/mol×K	722.40	Joback Method
dvisc	0.0040411	Pa×s	303.44	Joback Method
dvisc	0.0021881	Pa×s	339.65	Joback Method
dvisc	0.0013334	Pa×s	375.87	Joback Method
dvisc	0.0008865	Pa×s	412.09	Joback Method
dvisc	0.0006296	Pa×s	448.30	Joback Method
dvisc	0.0004706	Pa×s	484.51	Joback Method
dvisc	0.0003662	Pa×s	520.73	Joback Method
hvapt	54.90	kJ/mol	423.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.50 ± 0.50	K	0.90	NIST Webbook

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=C815689&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
hvapt: Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume