2,4-Pentanedione, 3-methyl-

Other names:	Methylacetylacetone
	3-Methyl-2,4-pentanedione
	3-Acetylbutan-2-one
	3-methylpentane-2,4-dione
Inchi:	InChI=1S/C6H10O2/c1-4(5(2)7)6(3)8/h4H,1-3H3
InchiKey:	GSOHKPVFCOWKPU-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CC(=O)C(C)C(C)=O
Mol. weight [g/mol]:	114.14
CAS:	815-57-6

Physical Properties

Property code	Value	Unit	Source
chl	-3353.20 ± 1.70	kJ/mol	NIST Webbook
gf	-260.64	kJ/mol	Joback Method
hf	-428.90	kJ/mol	NIST Webbook
hfl	-437.00 ± 1.90	kJ/mol	NIST Webbook
hfus	10.97	kJ/mol	Joback Method
hvap	48.50 ± 5.00	kJ/mol	NIST Webbook
ie	8.55	eV	NIST Webbook
log10ws	-0.65		Crippen Method
logp	0.801		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	897.00		NIST Webbook
rinpol	897.00		NIST Webbook
tb	442.15 ± 3.00	K	NIST Webbook
tb	446.20	K	NIST Webbook
tb	442.15 ± 3.00	K	NIST Webbook
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	238.49	J/mol×K	605.70	Joback Method
cpg	230.38	J/mol×K	573.36	Joback Method
cpg	221.86	J/mol×K	541.01	Joback Method
cpg	212.92	J/mol×K	508.67	Joback Method
cpg	203.55	J/mol×K	476.32	Joback Method
cpg	246.20	J/mol×K	638.05	Joback Method
dvisc	0.0003462	Pa×s	443.98	Joback Method
dvisc	0.0004487	Pa×s	410.36	Joback Method
dvisc	0.0006091	Pa×s	376.73	Joback Method
dvisc	0.0008780	Pa×s	343.11	Joback Method
dvisc	0.0013702	Pa×s	309.49	Joback Method
dvisc	0.0023833	Pa×s	275.86	Joback Method
dvisc	0.0048342	Pa×s	242.24	Joback Method

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=C815576&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume