2,4-Pentanedione, 3-ethyl-

Other names:	3-Acetyl-2-pentanone
	3-Ethyl-2,4-pentanedione
	3-Ethylacetylacetone
	3-ethylpentane-2,4-dione
Inchi:	InChI=1S/C7H12O2/c1-4-7(5(2)8)6(3)9/h7H,4H2,1-3H3
InchiKey:	GUARKOVVHJSMRW-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CCC(C(C)=O)C(C)=O
Mol. weight [g/mol]:	128.17
CAS:	1540-34-7

Physical Properties

Property code	Value	Unit	Source
gf	-252.22	kJ/mol	Joback Method
hf	-439.70	kJ/mol	NIST Webbook
hfus	13.56	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.191		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	466.86	K	Joback Method
tc	658.82	K	Joback Method
tf	253.51	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.52	J/mol×K	466.86	Joback Method
cpg	244.55	J/mol×K	498.85	Joback Method
cpg	255.07	J/mol×K	530.85	Joback Method
cpg	265.11	J/mol×K	562.84	Joback Method
cpg	274.67	J/mol×K	594.83	Joback Method

cpg	283.77	J/mol×K	626.83	Joback Method
cpg	292.41	J/mol×K	658.82	Joback Method
dvisc	0.0049833	Pa×s	253.51	Joback Method
dvisc	0.0024070	Pa×s	289.07	Joback Method
dvisc	0.0013635	Pa×s	324.63	Joback Method
dvisc	0.0008641	Pa×s	360.19	Joback Method
dvisc	0.0005944	Pa×s	395.74	Joback Method
dvisc	0.0004349	Pa×s	431.30	Joback Method
dvisc	0.0003337	Pa×s	466.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.70	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61017e+01
Coeff. B	-4.29528e+03
Coeff. C	-6.67090e+01
Temperature range (K), min.	338.32
Temperature range (K), max.	464.78

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1540347&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume